Full wwPDB X-ray Structure Validation Report (i)

May 3, 2025 – 08:50 AM EDT

PDB ID	:	3DKW / pdb_00003dkw
Title	:	Crystal Structure of DNR from Pseudomonas aeruginosa.
Authors	:	Giardina, G.
Deposited on	:	2008-06-26
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

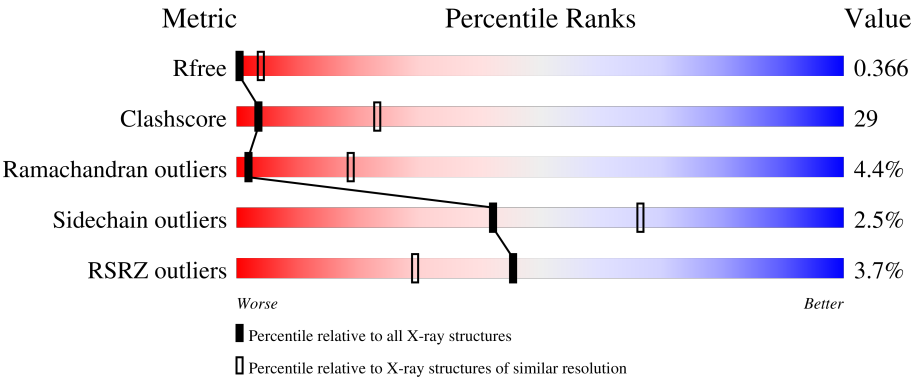
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	4% 54% 40% 6%
1	B	227	2% 68% 28% .
1	C	227	5% 56% 35% 7% .
1	D	227	3% 65% 29% 6%
1	E	227	4% 69% 29% .

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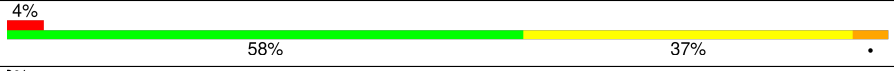
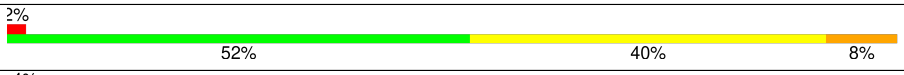
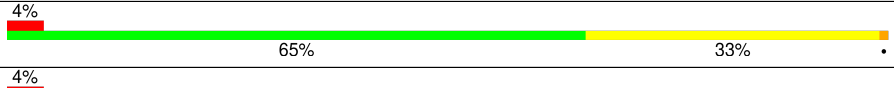
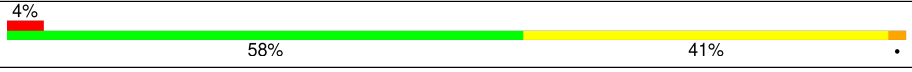
Mol	Chain	Length	Quality of chain
1	F	227	
1	G	227	
1	H	227	
1	I	227	
1	J	227	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18250 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNR protein.

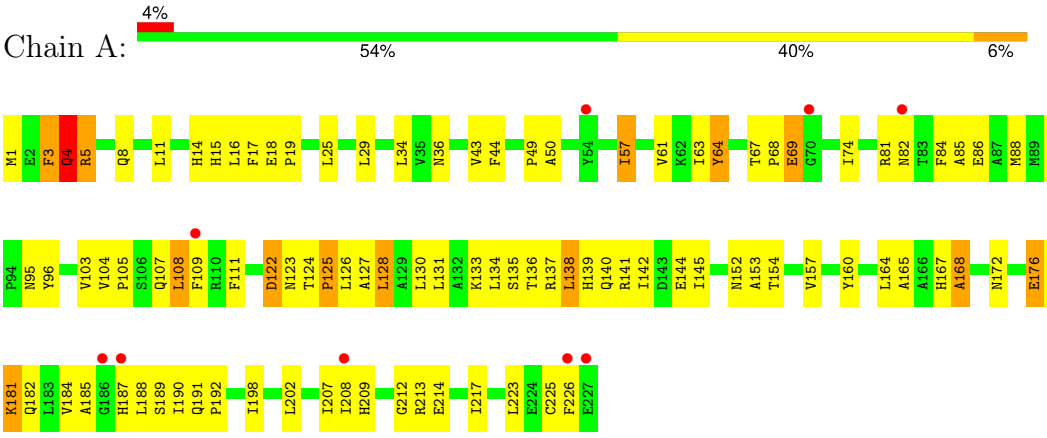
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	204	0	0
			1825	1158	325	334	8			
1	B	227	Total	C	N	O	S	354	0	0
			1825	1158	325	334	8			
1	C	227	Total	C	N	O	S	268	0	0
			1825	1158	325	334	8			
1	D	227	Total	C	N	O	S	483	0	0
			1825	1158	325	334	8			
1	E	227	Total	C	N	O	S	404	0	0
			1825	1158	325	334	8			
1	F	227	Total	C	N	O	S	417	0	0
			1825	1158	325	334	8			
1	G	227	Total	C	N	O	S	350	0	0
			1825	1158	325	334	8			
1	H	227	Total	C	N	O	S	352	0	0
			1825	1158	325	334	8			
1	I	227	Total	C	N	O	S	284	0	0
			1825	1158	325	334	8			
1	J	227	Total	C	N	O	S	206	0	0
			1825	1158	325	334	8			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

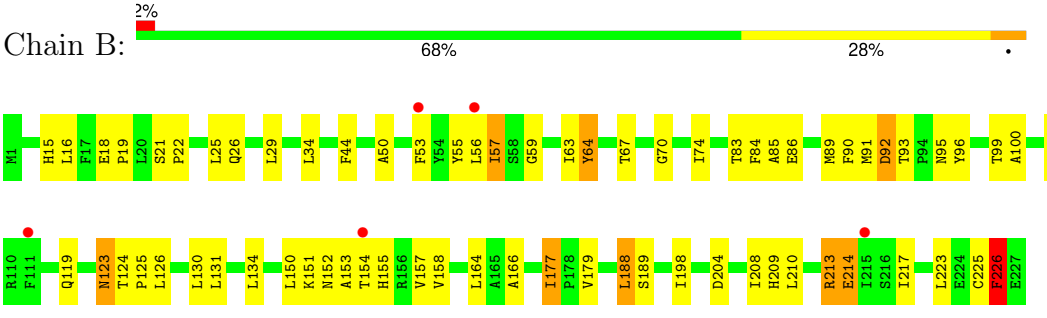
• Molecule 1: DNR protein

Chain A:



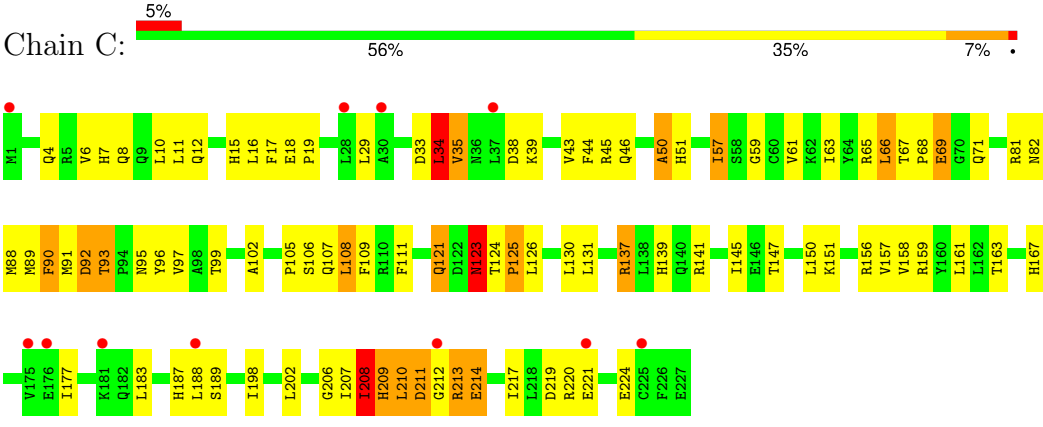
• Molecule 1: DNR protein

Chain B:



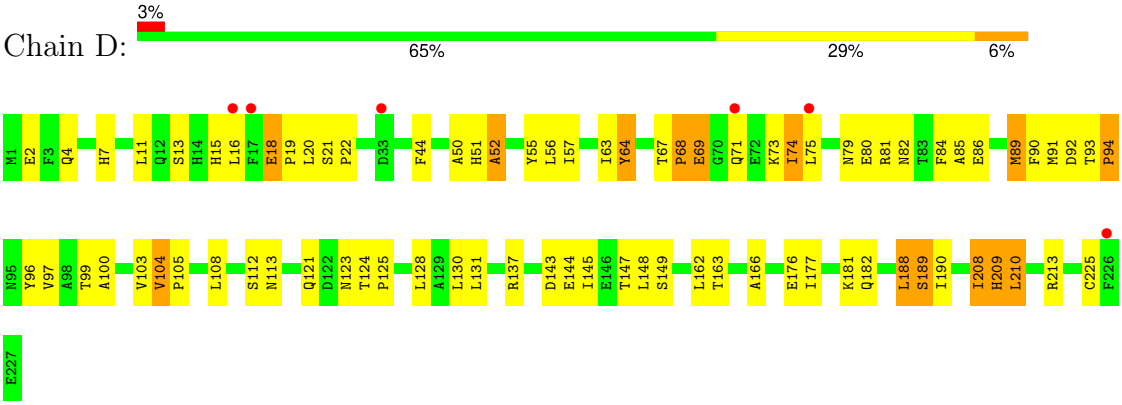
• Molecule 1: DNR protein

Chain C:



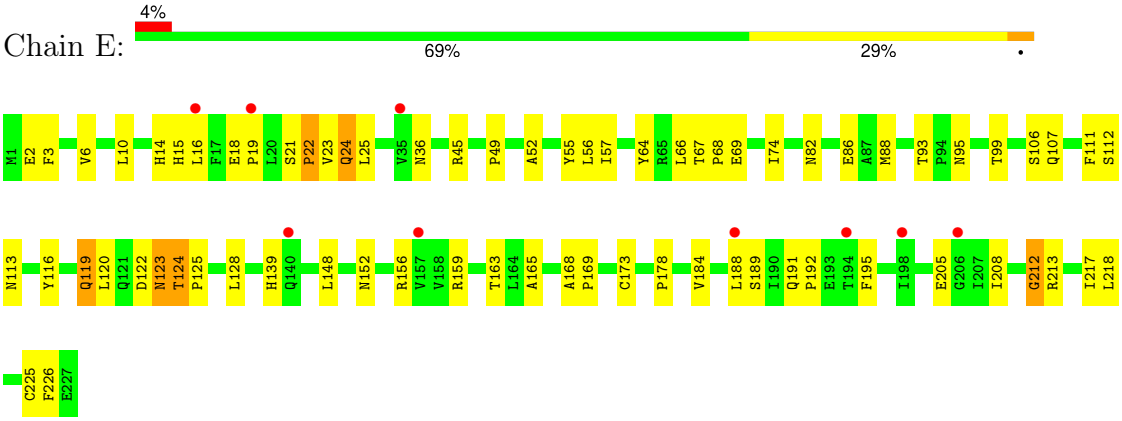
• Molecule 1: DNR protein

Chain D:



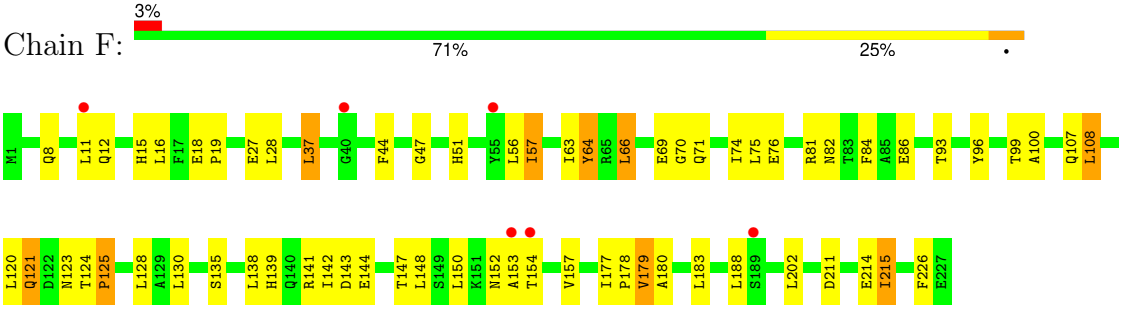
• Molecule 1: DNR protein

Chain E:



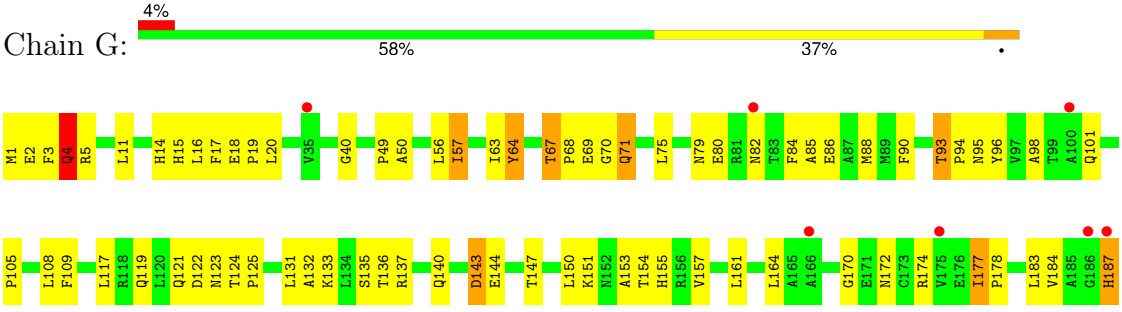
• Molecule 1: DNR protein

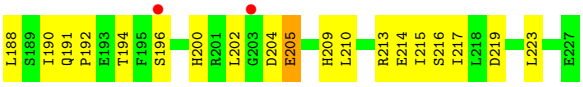
Chain F:



• Molecule 1: DNR protein

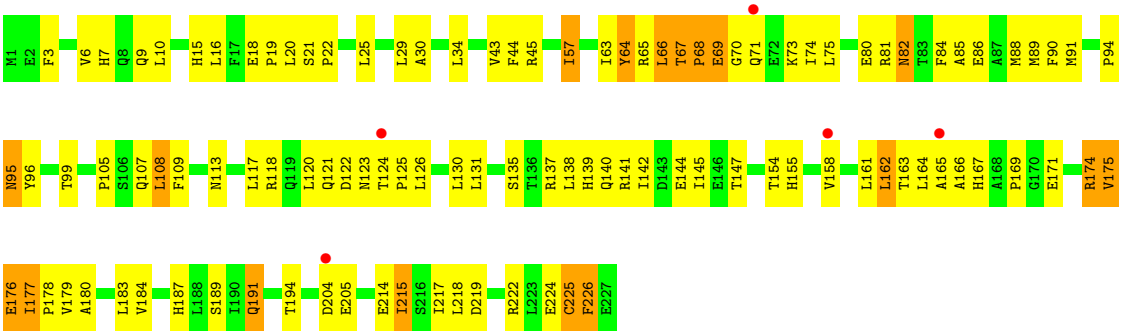
Chain G:





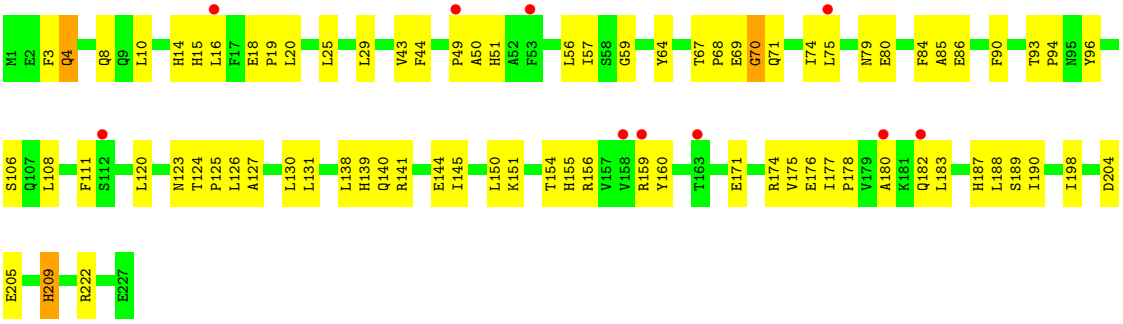
• Molecule 1: DNR protein

Chain H:



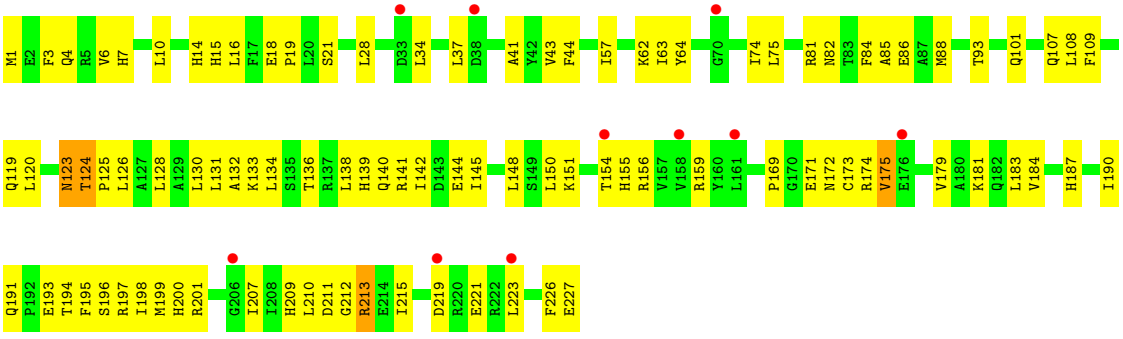
• Molecule 1: DNR protein

Chain I:



• Molecule 1: DNR protein

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	245.28Å 121.47Å 82.55Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	100.00 – 3.60 100.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (100.00-3.60) 96.7 (100.00-3.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.326 , 0.374 0.320 , 0.366	Depositor DCC
R_{free} test set	1359 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	79.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 70.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	18250	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.51	2/1861 (0.1%)	0.76	1/2520 (0.0%)
1	B	0.66	7/1861 (0.4%)	0.80	1/2520 (0.0%)
1	C	0.48	1/1861 (0.1%)	0.81	7/2520 (0.3%)
1	D	0.63	8/1861 (0.4%)	0.80	3/2520 (0.1%)
1	E	0.66	6/1861 (0.3%)	0.83	5/2520 (0.2%)
1	F	0.60	4/1861 (0.2%)	0.84	8/2520 (0.3%)
1	G	0.73	9/1861 (0.5%)	0.96	16/2520 (0.6%)
1	H	0.89	11/1861 (0.6%)	0.96	11/2520 (0.4%)
1	I	0.61	5/1861 (0.3%)	0.76	3/2520 (0.1%)
1	J	0.52	6/1861 (0.3%)	0.81	6/2520 (0.2%)
All	All	0.64	59/18610 (0.3%)	0.84	61/25200 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	4
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	9

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	226	PHE	C-O	18.09	1.46	1.24
1	H	171	GLU	C-O	15.31	1.40	1.24
1	G	187	HIS	CB-CG	-10.42	1.35	1.50
1	H	155	HIS	CB-CG	9.73	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	163	THR	CB-OG1	-9.33	1.28	1.43
1	D	181	LYS	C-O	9.06	1.35	1.24
1	I	177	ILE	CB-CG1	-8.44	1.36	1.53
1	I	222	ARG	C-O	-8.22	1.13	1.24
1	G	213	ARG	C-O	7.88	1.33	1.23
1	B	21	SER	CB-OG	-7.87	1.26	1.42
1	B	198	ILE	CB-CG1	7.86	1.69	1.53
1	E	226	PHE	C-N	7.85	1.44	1.33
1	I	190	ILE	CB-CG1	7.80	1.69	1.53
1	G	217	ILE	C-N	7.73	1.44	1.33
1	H	225	CYS	C-N	-7.68	1.23	1.33
1	E	205	GLU	C-N	7.53	1.44	1.33
1	F	66	LEU	C-N	7.20	1.48	1.33
1	D	2	GLU	C-N	7.04	1.42	1.33
1	A	209	HIS	CB-CG	-6.99	1.40	1.50
1	H	161	LEU	CB-CG	-6.96	1.39	1.53
1	H	187	HIS	C-N	-6.89	1.24	1.33
1	E	148	LEU	CB-CG	6.88	1.67	1.53
1	E	66	LEU	CB-CG	6.71	1.66	1.53
1	H	164	LEU	C-N	-6.57	1.24	1.33
1	A	182	GLN	CB-CG	6.42	1.71	1.52
1	H	73	LYS	CE-NZ	-6.26	1.30	1.49
1	J	211	ASP	C-O	6.07	1.31	1.24
1	J	219	ASP	CB-CG	6.03	1.67	1.52
1	D	162	LEU	CB-CG	6.00	1.65	1.53
1	G	223	LEU	CB-CG	-5.97	1.41	1.53
1	G	205	GLU	C-O	-5.88	1.16	1.24
1	H	177	ILE	CB-CG1	-5.80	1.41	1.53
1	D	130	LEU	CB-CG	5.80	1.65	1.53
1	B	226	PHE	C-N	5.56	1.41	1.33
1	G	205	GLU	C-N	5.55	1.41	1.33
1	H	215	ILE	C-N	5.53	1.41	1.33
1	F	27	GLU	CA-CB	5.51	1.62	1.53
1	I	187	HIS	CB-CG	-5.51	1.42	1.50
1	D	163	THR	CB-OG1	-5.38	1.35	1.43
1	B	210	LEU	C-N	-5.37	1.25	1.33
1	J	209	HIS	C-N	-5.36	1.26	1.33
1	D	112	SER	CB-OG	-5.35	1.31	1.42
1	I	209	HIS	C-O	5.35	1.30	1.23
1	E	86	GLU	CB-CG	-5.32	1.36	1.52
1	B	213	ARG	CB-CG	5.32	1.68	1.52
1	G	93	THR	CB-OG1	5.30	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	96	TYR	CB-CG	5.29	1.63	1.51
1	J	209	HIS	CB-CG	-5.28	1.42	1.50
1	G	135	SER	CB-OG	-5.27	1.31	1.42
1	B	188	LEU	CB-CG	5.19	1.63	1.53
1	C	224	GLU	CG-CD	5.17	1.65	1.52
1	J	21	SER	CB-OG	-5.17	1.31	1.42
1	E	128	LEU	CB-CG	5.16	1.63	1.53
1	J	210	LEU	C-O	-5.08	1.18	1.24
1	B	130	LEU	CB-CG	5.05	1.63	1.53
1	D	213	ARG	CA-CB	-5.03	1.46	1.53
1	D	209	HIS	C-O	5.02	1.30	1.23
1	F	28	LEU	CG-CD1	-5.00	1.36	1.52
1	G	174	ARG	CB-CG	5.00	1.67	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	215	ILE	O-C-N	-10.75	111.59	123.10
1	H	164	LEU	CA-C-N	10.72	142.01	121.54
1	H	164	LEU	C-N-CA	10.72	142.01	121.54
1	D	208	ILE	CA-C-O	-9.41	110.60	120.39
1	H	155	HIS	CA-CB-CG	-9.41	104.39	113.80
1	H	164	LEU	O-C-N	-8.43	111.38	122.59
1	B	204	ASP	CA-CB-CG	8.27	120.87	112.60
1	G	5	ARG	N-CA-CB	7.94	123.92	110.49
1	F	96	TYR	CB-CG-CD2	-7.92	108.93	120.80
1	H	225	CYS	O-C-N	-7.89	112.14	122.39
1	F	96	TYR	CB-CG-CD1	7.83	132.55	120.80
1	F	37	LEU	CD1-CG-CD2	7.75	127.86	110.80
1	G	177	ILE	CA-C-N	-7.69	110.23	119.84
1	G	177	ILE	C-N-CA	-7.69	110.23	119.84
1	J	226	PHE	CA-CB-CG	7.50	121.30	113.80
1	E	205	GLU	O-C-N	7.30	131.71	122.37
1	F	96	TYR	CA-CB-CG	-7.08	101.15	113.90
1	H	191	GLN	CA-C-N	-7.06	111.01	119.84
1	H	191	GLN	C-N-CA	-7.06	111.01	119.84
1	G	213	ARG	CA-C-N	-7.01	112.28	122.44
1	G	213	ARG	C-N-CA	-7.01	112.28	122.44
1	F	211	ASP	CA-CB-CG	6.97	119.57	112.60
1	J	187	HIS	CA-CB-CG	6.87	120.67	113.80
1	C	137	ARG	CG-CD-NE	6.87	127.11	112.00
1	D	210	LEU	O-C-N	-6.85	115.25	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	95	ASN	CA-CB-CG	6.76	119.36	112.60
1	G	217	ILE	O-C-N	6.66	130.56	121.90
1	D	209	HIS	CA-C-O	-6.62	113.68	121.16
1	G	217	ILE	CA-C-N	-6.55	111.63	121.72
1	G	217	ILE	C-N-CA	-6.55	111.63	121.72
1	F	226	PHE	CA-CB-CG	-6.52	107.28	113.80
1	G	204	ASP	CA-C-O	6.35	127.23	119.11
1	H	187	HIS	CA-C-O	-6.33	113.86	121.34
1	H	174	ARG	CA-CB-CG	6.33	126.76	114.10
1	C	8	GLN	CA-CB-CG	6.30	126.70	114.10
1	G	214	GLU	CA-CB-CG	6.18	126.46	114.10
1	F	28	LEU	CB-CG-CD1	6.12	129.06	110.70
1	G	204	ASP	O-C-N	-6.04	113.61	122.43
1	J	219	ASP	CA-CB-CG	-5.96	106.64	112.60
1	I	177	ILE	CA-CB-CG1	5.87	120.38	110.40
1	A	137	ARG	CA-CB-CG	-5.82	102.46	114.10
1	E	165	ALA	N-CA-C	-5.81	106.28	113.19
1	E	226	PHE	CB-CA-C	-5.76	102.14	111.06
1	C	171	GLU	CA-C-N	-5.71	111.23	122.02
1	C	171	GLU	C-N-CA	-5.71	111.23	122.02
1	F	141	ARG	CA-CB-CG	-5.58	102.95	114.10
1	J	209	HIS	O-C-N	-5.50	116.23	123.16
1	G	4	GLN	CA-CB-CG	-5.47	103.16	114.10
1	I	222	ARG	CA-C-O	-5.44	112.69	119.38
1	I	182	GLN	CA-CB-CG	5.40	124.90	114.10
1	H	177	ILE	CA-CB-CG1	5.40	119.58	110.40
1	G	143	ASP	CA-CB-CG	-5.33	107.27	112.60
1	E	82	ASN	CA-CB-CG	5.33	117.93	112.60
1	C	167	HIS	O-C-N	5.30	129.12	122.86
1	E	226	PHE	CA-CB-CG	-5.29	108.51	113.80
1	G	71	GLN	CB-CG-CD	5.26	121.54	112.60
1	J	212	GLY	CA-C-N	5.19	131.45	121.54
1	J	212	GLY	C-N-CA	5.19	131.45	121.54
1	G	71	GLN	CA-CB-CG	-5.16	103.79	114.10
1	G	187	HIS	CA-CB-CG	5.05	118.85	113.80
1	C	183	LEU	CB-CG-CD1	-5.00	95.69	110.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	D	182	GLN	Mainchain
1	D	208	ILE	Mainchain
1	D	209	HIS	Mainchain
1	D	210	LEU	Mainchain
1	F	93	THR	Mainchain
1	G	205	GLU	Mainchain
1	H	215	ILE	Mainchain
1	I	209	HIS	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1825	0	1837	117	1
1	B	1825	0	1837	83	0
1	C	1825	0	1837	118	1
1	D	1825	0	1837	85	0
1	E	1825	0	1837	76	0
1	F	1825	0	1837	68	0
1	G	1825	0	1837	87	0
1	H	1825	0	1836	100	1
1	I	1825	0	1837	94	1
1	J	1825	0	1837	106	0
All	All	18250	0	18369	830	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (830) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:124:THR:OG1	1:J:125:PRO:HD3	1.24	1.34
1:E:22:PRO:O	1:E:25:LEU:HD13	1.12	1.30
1:D:103:VAL:O	1:D:104:VAL:CG1	1.81	1.28
1:A:152:ASN:OD1	1:B:152:ASN:OD1	1.56	1.24
1:I:138:LEU:HD13	1:J:138:LEU:CD2	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:THR:CG2	1:C:68:PRO:HD2	1.72	1.19
1:G:190:ILE:HG22	1:G:192:PRO:CD	1.75	1.16
1:A:131:LEU:HD23	1:B:131:LEU:CD2	1.76	1.15
1:F:179:VAL:HG12	1:F:180:ALA:H	1.07	1.14
1:A:213:ARG:NH1	1:H:30:ALA:HA	1.63	1.13
1:E:21:SER:HB2	1:E:22:PRO:HD2	1.19	1.13
1:D:103:VAL:O	1:D:104:VAL:HG12	0.96	1.13
1:A:131:LEU:HD23	1:B:131:LEU:HD23	1.30	1.12
1:A:131:LEU:CD2	1:B:131:LEU:HD23	1.78	1.12
1:A:131:LEU:CD2	1:B:131:LEU:CD2	2.26	1.12
1:G:131:LEU:CD2	1:H:131:LEU:HD23	1.80	1.12
1:G:131:LEU:HD23	1:H:131:LEU:CD2	1.80	1.12
1:C:131:LEU:HD23	1:D:131:LEU:HD23	1.30	1.12
1:D:89:MET:HE3	1:D:89:MET:HA	1.31	1.12
1:C:145:ILE:HG12	1:D:145:ILE:HD11	1.22	1.11
1:J:123:ASN:ND2	1:J:126:LEU:HD12	1.67	1.10
1:J:123:ASN:O	1:J:124:THR:OG1	1.66	1.08
1:D:124:THR:OG1	1:D:125:PRO:HD3	1.50	1.08
1:G:20:LEU:CD2	1:G:119:GLN:HE22	1.66	1.08
1:G:20:LEU:HD21	1:G:119:GLN:HE22	1.18	1.08
1:C:67:THR:HG22	1:C:68:PRO:HD2	1.29	1.07
1:A:138:LEU:HD23	1:A:138:LEU:O	1.54	1.06
1:B:208:ILE:HG22	1:B:209:HIS:H	0.95	1.06
1:H:67:THR:HB	1:H:68:PRO:HD2	1.37	1.06
1:E:124:THR:HB	1:E:125:PRO:HD3	1.31	1.05
1:G:131:LEU:HD23	1:H:131:LEU:HD23	1.10	1.05
1:F:202:LEU:O	1:F:202:LEU:HD23	1.58	1.04
1:J:64:TYR:HB3	1:J:74:ILE:HD13	1.37	1.04
1:I:138:LEU:CD1	1:J:138:LEU:HD23	1.87	1.04
1:C:107:GLN:C	1:C:108:LEU:HD12	1.83	1.03
1:H:64:TYR:HB3	1:H:74:ILE:HD13	1.40	1.03
1:F:107:GLN:C	1:F:108:LEU:HD12	1.84	1.02
1:G:190:ILE:CG2	1:G:192:PRO:HD2	1.89	1.02
1:I:131:LEU:CD2	1:J:131:LEU:HD23	1.90	1.02
1:H:81:ARG:C	1:H:82:ASN:HD22	1.68	1.01
1:H:124:THR:N	1:H:125:PRO:HD2	1.75	1.01
1:E:22:PRO:O	1:E:25:LEU:CD1	2.08	1.01
1:E:152:ASN:OD1	1:F:152:ASN:ND2	1.95	1.00
1:J:14:HIS:O	1:J:18:GLU:HG3	1.59	1.00
1:H:158:VAL:O	1:H:162:LEU:HB2	1.62	0.99
1:B:208:ILE:HG22	1:B:209:HIS:N	1.77	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:LEU:HD13	1:J:138:LEU:HD23	1.03	0.99
1:C:145:ILE:CG1	1:D:145:ILE:HD11	1.93	0.98
1:G:131:LEU:CD2	1:H:131:LEU:CD2	2.38	0.98
1:B:99:THR:HG22	1:B:100:ALA:H	1.22	0.98
1:J:123:ASN:HD22	1:J:126:LEU:HD12	1.19	0.98
1:J:130:LEU:HD23	1:J:130:LEU:O	1.63	0.98
1:D:99:THR:HG22	1:D:100:ALA:H	1.28	0.97
1:H:66:LEU:O	1:H:67:THR:OG1	1.81	0.97
1:A:107:GLN:C	1:A:108:LEU:HD12	1.88	0.97
1:I:131:LEU:HD23	1:J:131:LEU:HD23	1.44	0.96
1:A:88:MET:HE3	1:A:93:THR:OG1	1.65	0.96
1:B:107:GLN:C	1:B:108:LEU:HD12	1.89	0.96
1:B:53:PHE:CE1	1:B:89:MET:CE	2.48	0.96
1:J:124:THR:OG1	1:J:125:PRO:CD	2.14	0.95
1:F:99:THR:HG22	1:F:100:ALA:H	1.30	0.95
1:C:208:ILE:C	1:C:208:ILE:HD12	1.92	0.95
1:G:20:LEU:CD2	1:G:119:GLN:NE2	2.29	0.94
1:A:181:LYS:O	1:A:184:VAL:HG12	1.65	0.94
1:C:131:LEU:HD23	1:D:131:LEU:CD2	1.98	0.94
1:C:18:GLU:HB3	1:C:19:PRO:HD3	1.47	0.94
1:D:148:LEU:HD12	1:D:149:SER:N	1.83	0.93
1:H:123:ASN:C	1:H:125:PRO:HD2	1.94	0.93
1:H:88:MET:HE1	1:H:96:TYR:HA	1.51	0.92
1:B:123:ASN:HD21	1:B:126:LEU:HB2	1.33	0.92
1:B:53:PHE:CD1	1:B:89:MET:CE	2.53	0.92
1:E:6:VAL:HG11	1:H:7:HIS:CE1	2.04	0.92
1:G:190:ILE:HG22	1:G:192:PRO:HD2	0.96	0.92
1:C:145:ILE:HG12	1:D:145:ILE:CD1	2.00	0.92
1:I:156:ARG:HB2	1:I:188:LEU:HD21	1.52	0.92
1:D:103:VAL:C	1:D:104:VAL:HG12	1.95	0.91
1:I:156:ARG:HB2	1:I:188:LEU:CD2	2.00	0.91
1:E:123:ASN:ND2	1:F:123:ASN:O	2.04	0.91
1:C:121:GLN:NE2	1:E:36:ASN:HD21	1.69	0.91
1:D:89:MET:HE1	1:D:113:ASN:HB3	1.49	0.91
1:I:124:THR:N	1:I:125:PRO:HD2	1.86	0.90
1:C:147:THR:O	1:C:151:LYS:HG3	1.69	0.90
1:E:21:SER:HB2	1:E:22:PRO:CD	2.01	0.90
1:C:10:LEU:HD23	1:I:10:LEU:HD23	1.52	0.90
1:A:128:LEU:HD21	1:B:90:PHE:O	1.71	0.90
1:H:107:GLN:C	1:H:108:LEU:HD12	1.96	0.90
1:A:131:LEU:CD2	1:B:131:LEU:HD21	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASN:C	1:A:125:PRO:HD2	1.97	0.89
1:C:67:THR:HG22	1:C:68:PRO:CD	2.02	0.89
1:H:130:LEU:HD23	1:H:130:LEU:O	1.73	0.89
1:A:68:PRO:O	1:A:69:GLU:HB2	1.68	0.89
1:C:211:ASP:CG	1:C:214:GLU:O	2.15	0.89
1:C:19:PRO:HG2	1:C:130:LEU:HD23	1.54	0.89
1:B:208:ILE:CG2	1:B:209:HIS:H	1.81	0.89
1:B:53:PHE:CE1	1:B:89:MET:HE1	2.08	0.88
1:G:20:LEU:HD21	1:G:119:GLN:NE2	1.86	0.88
1:B:57:ILE:HD12	1:B:57:ILE:N	1.89	0.88
1:C:210:LEU:HD12	1:C:210:LEU:H	1.39	0.88
1:A:128:LEU:HD23	1:A:128:LEU:O	1.75	0.87
1:I:131:LEU:CD2	1:J:131:LEU:CD2	2.53	0.87
1:C:67:THR:HG23	1:C:68:PRO:HD2	1.53	0.87
1:E:23:VAL:O	1:E:25:LEU:N	2.08	0.87
1:A:131:LEU:HD21	1:B:131:LEU:CD2	2.04	0.87
1:C:10:LEU:HD23	1:I:10:LEU:CD2	2.05	0.86
1:J:10:LEU:HD23	1:J:10:LEU:H	1.41	0.86
1:C:131:LEU:CD2	1:D:131:LEU:HD23	2.05	0.86
1:F:179:VAL:HG12	1:F:180:ALA:N	1.89	0.86
1:F:64:TYR:HB3	1:F:74:ILE:HD13	1.57	0.86
1:B:124:THR:HG22	1:B:125:PRO:HD3	1.58	0.86
1:B:124:THR:CG2	1:B:125:PRO:HD3	2.05	0.86
1:C:208:ILE:HG22	1:C:217:ILE:HA	1.57	0.86
1:A:138:LEU:HD23	1:A:138:LEU:C	2.01	0.86
1:A:139:HIS:NE2	1:B:86:GLU:OE2	2.08	0.85
1:A:128:LEU:HD23	1:A:128:LEU:C	2.02	0.85
1:F:99:THR:HG22	1:F:100:ALA:N	1.93	0.84
1:I:124:THR:H	1:I:125:PRO:HD2	1.39	0.84
1:C:139:HIS:CE1	1:D:86:GLU:OE2	2.30	0.84
1:B:99:THR:HG22	1:B:100:ALA:N	1.91	0.84
1:G:57:ILE:HD12	1:G:57:ILE:N	1.93	0.84
1:I:131:LEU:HD23	1:J:131:LEU:CD2	2.07	0.83
1:B:91:MET:O	1:B:93:THR:HG23	1.77	0.83
1:F:57:ILE:N	1:F:57:ILE:HD12	1.93	0.83
1:C:131:LEU:CD2	1:D:131:LEU:CD2	2.57	0.83
1:F:124:THR:N	1:F:125:PRO:CD	2.41	0.83
1:D:89:MET:HE3	1:D:89:MET:CA	2.07	0.83
1:E:6:VAL:HG11	1:H:7:HIS:HE1	1.43	0.82
1:C:57:ILE:N	1:C:57:ILE:HD12	1.95	0.82
1:A:131:LEU:HD23	1:B:131:LEU:HD21	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:THR:HG22	1:D:100:ALA:N	1.94	0.81
1:B:34:LEU:HD11	1:B:107:GLN:HE21	1.44	0.81
1:H:174:ARG:O	1:H:175:VAL:HB	1.81	0.81
1:H:124:THR:N	1:H:125:PRO:CD	2.44	0.81
1:E:21:SER:CB	1:E:22:PRO:HD2	2.07	0.80
1:A:190:ILE:HD12	1:A:190:ILE:C	2.06	0.80
1:C:123:ASN:O	1:C:124:THR:OG1	2.00	0.80
1:J:64:TYR:HB3	1:J:74:ILE:CD1	2.12	0.80
1:I:188:LEU:O	1:I:189:SER:OG	1.98	0.79
1:H:57:ILE:N	1:H:57:ILE:HD12	1.97	0.79
1:A:190:ILE:HD12	1:A:190:ILE:O	1.81	0.79
1:C:211:ASP:OD2	1:C:214:GLU:O	2.01	0.79
1:H:64:TYR:HB3	1:H:74:ILE:CD1	2.12	0.79
1:I:156:ARG:CB	1:I:188:LEU:CD2	2.61	0.79
1:G:191:GLN:N	1:G:192:PRO:HD2	1.98	0.78
1:E:124:THR:HB	1:E:125:PRO:CD	2.12	0.78
1:H:66:LEU:C	1:H:67:THR:HG1	1.90	0.78
1:F:215:ILE:HD12	1:F:215:ILE:N	1.97	0.78
1:A:95:ASN:ND2	1:D:225:CYS:SG	2.57	0.78
1:C:10:LEU:CD2	1:I:10:LEU:CD2	2.62	0.77
1:C:67:THR:CG2	1:C:68:PRO:CD	2.57	0.77
1:C:10:LEU:CD2	1:I:10:LEU:HD23	2.14	0.77
1:B:91:MET:O	1:B:93:THR:N	2.17	0.77
1:C:209:HIS:O	1:C:210:LEU:O	2.02	0.77
1:I:156:ARG:CB	1:I:188:LEU:HD21	2.15	0.77
1:A:57:ILE:N	1:A:57:ILE:HD12	1.99	0.76
1:A:14:HIS:O	1:A:18:GLU:HG3	1.85	0.76
1:B:123:ASN:ND2	1:B:126:LEU:HB2	1.99	0.76
1:F:124:THR:N	1:F:125:PRO:HD2	1.99	0.76
1:E:21:SER:O	1:E:23:VAL:N	2.20	0.75
1:H:15:HIS:HB3	1:H:137:ARG:HD2	1.68	0.75
1:C:210:LEU:O	1:C:211:ASP:CB	2.34	0.75
1:C:208:ILE:O	1:C:209:HIS:HB3	1.87	0.75
1:C:208:ILE:C	1:C:208:ILE:CD1	2.59	0.74
1:J:194:THR:O	1:J:198:ILE:HG13	1.87	0.74
1:B:99:THR:CG2	1:B:100:ALA:H	2.00	0.74
1:H:81:ARG:O	1:H:82:ASN:ND2	2.19	0.74
1:F:19:PRO:HG2	1:F:130:LEU:HD23	1.70	0.74
1:C:139:HIS:HE1	1:D:86:GLU:OE2	1.69	0.74
1:I:69:GLU:OE1	1:I:69:GLU:O	2.05	0.74
1:C:208:ILE:O	1:C:209:HIS:CB	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:VAL:C	1:E:25:LEU:H	1.94	0.73
1:J:140:GLN:O	1:J:144:GLU:HG3	1.88	0.73
1:C:210:LEU:O	1:C:211:ASP:HB2	1.86	0.73
1:H:67:THR:HB	1:H:68:PRO:CD	2.17	0.73
1:J:181:LYS:HB2	1:J:184:VAL:CG2	2.19	0.73
1:G:20:LEU:HD23	1:G:119:GLN:NE2	2.03	0.73
1:I:131:LEU:HD21	1:J:131:LEU:HD23	1.70	0.72
1:B:123:ASN:C	1:B:123:ASN:OD1	2.33	0.72
1:C:156:ARG:HG2	1:C:188:LEU:HD13	1.70	0.72
1:I:131:LEU:HD21	1:J:131:LEU:CD2	2.19	0.72
1:B:64:TYR:HB3	1:B:74:ILE:HD13	1.72	0.72
1:I:124:THR:N	1:I:125:PRO:CD	2.52	0.72
1:J:207:ILE:HG22	1:J:207:ILE:O	1.89	0.71
1:H:34:LEU:HD21	1:H:107:GLN:HE21	1.54	0.71
1:E:18:GLU:HB3	1:E:19:PRO:HD3	1.73	0.71
1:C:121:GLN:NE2	1:E:36:ASN:ND2	2.39	0.71
1:D:108:LEU:HD12	1:D:108:LEU:O	1.90	0.71
1:J:123:ASN:ND2	1:J:126:LEU:CD1	2.52	0.71
1:A:4:GLN:O	1:A:5:ARG:HB2	1.92	0.70
1:F:177:ILE:N	1:F:178:PRO:HA	2.05	0.70
1:C:50:ALA:HA	1:C:96:TYR:CE2	2.26	0.70
1:A:64:TYR:HB3	1:A:74:ILE:HD13	1.74	0.70
1:I:70:GLY:O	1:I:71:GLN:HG2	1.92	0.70
1:J:107:GLN:C	1:J:108:LEU:HD12	2.16	0.70
1:D:21:SER:HB2	1:D:22:PRO:HD2	1.74	0.69
1:E:120:LEU:CD2	1:F:128:LEU:HD21	2.23	0.69
1:F:179:VAL:CG1	1:F:180:ALA:H	1.91	0.69
1:J:174:ARG:O	1:J:175:VAL:HB	1.92	0.69
1:G:184:VAL:HG22	1:G:194:THR:HG21	1.73	0.69
1:J:10:LEU:H	1:J:10:LEU:CD2	2.06	0.69
1:A:8:GLN:HG3	1:A:25:LEU:CD2	2.23	0.69
1:A:124:THR:N	1:A:125:PRO:HD2	2.08	0.69
1:F:99:THR:CG2	1:F:100:ALA:H	2.04	0.69
1:A:92:ASP:HB2	1:C:187:HIS:CD2	2.27	0.69
1:E:88:MET:HE3	1:E:93:THR:HG21	1.73	0.69
1:G:86:GLU:OE2	1:H:139:HIS:NE2	2.24	0.68
1:G:124:THR:OG1	1:G:125:PRO:HD3	1.93	0.68
1:G:150:LEU:O	1:G:154:THR:HG23	1.93	0.68
1:H:218:LEU:O	1:H:222:ARG:HG3	1.93	0.68
1:B:53:PHE:CD1	1:B:89:MET:HE2	2.27	0.68
1:C:108:LEU:HD12	1:C:108:LEU:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:GLN:NE2	1:I:25:LEU:HD13	2.08	0.68
1:I:14:HIS:O	1:I:18:GLU:HG3	1.91	0.68
1:A:108:LEU:HD12	1:A:108:LEU:N	2.09	0.68
1:F:138:LEU:O	1:F:142:ILE:HG13	1.93	0.68
1:A:134:LEU:HD23	1:B:134:LEU:HD23	1.75	0.68
1:H:108:LEU:HD12	1:H:108:LEU:N	2.09	0.68
1:J:123:ASN:O	1:J:124:THR:CB	2.40	0.68
1:B:34:LEU:HD11	1:B:107:GLN:NE2	2.08	0.68
1:F:108:LEU:HD12	1:F:108:LEU:N	2.08	0.68
1:D:89:MET:HA	1:D:89:MET:CE	2.18	0.68
1:F:202:LEU:O	1:F:202:LEU:CD2	2.39	0.68
1:I:124:THR:H	1:I:125:PRO:CD	2.06	0.68
1:D:93:THR:N	1:D:94:PRO:HD3	2.10	0.67
1:E:64:TYR:HB3	1:E:74:ILE:HD13	1.76	0.67
1:A:213:ARG:HH11	1:H:30:ALA:HA	1.58	0.67
1:C:50:ALA:O	1:C:51:HIS:HB2	1.94	0.67
1:E:88:MET:CE	1:E:93:THR:HG21	2.24	0.67
1:F:120:LEU:O	1:F:121:GLN:C	2.38	0.67
1:C:209:HIS:O	1:C:210:LEU:C	2.38	0.67
1:J:64:TYR:CB	1:J:74:ILE:HD13	2.21	0.67
1:I:171:GLU:OE1	1:I:174:ARG:HD2	1.93	0.67
1:A:152:ASN:CG	1:B:152:ASN:OD1	2.37	0.67
1:B:124:THR:N	1:B:125:PRO:CD	2.58	0.67
1:C:81:ARG:O	1:C:82:ASN:OD1	2.11	0.67
1:B:63:ILE:O	1:B:64:TYR:CG	2.48	0.67
1:J:75:LEU:N	1:J:75:LEU:HD12	2.09	0.67
1:H:64:TYR:CB	1:H:74:ILE:HD13	2.23	0.67
1:I:90:PHE:HB2	1:J:132:ALA:HB2	1.77	0.67
1:D:81:ARG:O	1:D:82:ASN:OD1	2.13	0.66
1:D:15:HIS:HB3	1:D:137:ARG:NE	2.11	0.66
1:A:131:LEU:HD21	1:B:131:LEU:HD23	1.62	0.66
1:A:164:LEU:C	1:A:164:LEU:HD12	2.21	0.66
1:E:122:ASP:OD1	1:E:123:ASN:N	2.27	0.66
1:J:181:LYS:HB2	1:J:184:VAL:HG23	1.77	0.66
1:D:143:ASP:O	1:D:147:THR:HG23	1.96	0.66
1:G:131:LEU:HD21	1:H:131:LEU:CD2	2.24	0.66
1:B:18:GLU:HB3	1:B:19:PRO:HD3	1.76	0.66
1:A:164:LEU:HD12	1:A:165:ALA:N	2.11	0.66
1:C:207:ILE:O	1:C:208:ILE:HG23	1.96	0.66
1:C:12:GLN:O	1:C:18:GLU:OE1	2.14	0.66
1:C:124:THR:HB	1:C:125:PRO:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:GLU:HB3	1:D:19:PRO:HD3	1.77	0.66
1:G:121:GLN:O	1:G:122:ASP:HB2	1.95	0.66
1:H:94:PRO:C	1:H:95:ASN:HD22	2.03	0.66
1:H:95:ASN:HD22	1:H:95:ASN:N	1.94	0.65
1:C:210:LEU:H	1:C:210:LEU:CD1	2.09	0.65
1:A:29:LEU:HD23	1:A:111:PHE:HE2	1.60	0.65
1:G:20:LEU:HD23	1:G:119:GLN:HE22	1.54	0.65
1:D:99:THR:CG2	1:D:100:ALA:H	2.04	0.65
1:G:131:LEU:CD2	1:H:131:LEU:HD21	2.24	0.65
1:B:53:PHE:CE1	1:B:89:MET:HE2	2.29	0.65
1:I:56:LEU:HA	1:I:108:LEU:HD23	1.77	0.65
1:D:123:ASN:HD22	1:D:125:PRO:HD2	1.61	0.65
1:E:52:ALA:HB2	1:E:112:SER:HA	1.78	0.65
1:A:57:ILE:HD11	1:A:109:PHE:CD1	2.32	0.64
1:C:208:ILE:CG2	1:C:217:ILE:HA	2.27	0.64
1:I:159:ARG:CZ	1:J:159:ARG:HD2	2.26	0.64
1:H:18:GLU:N	1:H:19:PRO:HD2	2.11	0.64
1:B:53:PHE:CD1	1:B:89:MET:HE3	2.31	0.64
1:C:207:ILE:O	1:C:208:ILE:CG2	2.45	0.64
1:I:138:LEU:CD1	1:J:138:LEU:CD2	2.57	0.64
1:J:18:GLU:OE1	1:J:133:LYS:HD2	1.97	0.64
1:D:89:MET:HE1	1:D:113:ASN:CB	2.25	0.64
1:B:57:ILE:N	1:B:57:ILE:CD1	2.59	0.63
1:I:20:LEU:HB2	1:I:25:LEU:HD21	1.79	0.63
1:E:23:VAL:C	1:E:25:LEU:N	2.51	0.63
1:G:40:GLY:HA2	1:G:101:GLN:HE21	1.62	0.63
1:I:64:TYR:HB3	1:I:74:ILE:HD13	1.78	0.63
1:E:52:ALA:HA	1:E:113:ASN:OD1	1.99	0.63
1:G:57:ILE:N	1:G:57:ILE:CD1	2.62	0.63
1:A:128:LEU:C	1:A:128:LEU:CD2	2.71	0.63
1:E:120:LEU:HD21	1:F:128:LEU:CD2	2.29	0.63
1:A:167:HIS:O	1:A:168:ALA:HB3	1.96	0.63
1:F:57:ILE:N	1:F:57:ILE:CD1	2.61	0.63
1:J:10:LEU:HD23	1:J:10:LEU:N	2.13	0.63
1:A:8:GLN:HG3	1:A:25:LEU:HD21	1.81	0.62
1:F:56:LEU:C	1:F:57:ILE:HD12	2.24	0.62
1:D:18:GLU:H	1:D:19:PRO:CD	2.13	0.62
1:A:34:LEU:HD11	1:A:107:GLN:HE21	1.65	0.62
1:I:18:GLU:N	1:I:19:PRO:HD2	2.13	0.62
1:D:20:LEU:HD12	1:D:20:LEU:N	2.15	0.62
1:D:44:PHE:H	1:D:100:ALA:HB3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:LEU:HD21	1:F:128:LEU:HD21	1.80	0.62
1:G:191:GLN:N	1:G:192:PRO:CD	2.62	0.62
1:H:34:LEU:HD21	1:H:107:GLN:NE2	2.15	0.61
1:A:18:GLU:HB2	1:A:19:PRO:HD3	1.81	0.61
1:A:138:LEU:C	1:A:138:LEU:CD2	2.72	0.61
1:I:124:THR:CG2	1:I:125:PRO:HD3	2.29	0.61
1:A:190:ILE:C	1:A:190:ILE:CD1	2.70	0.61
1:C:57:ILE:N	1:C:57:ILE:CD1	2.63	0.61
1:E:212:GLY:O	1:E:213:ARG:HB2	1.99	0.61
1:F:124:THR:H	1:F:125:PRO:CD	2.11	0.61
1:B:164:LEU:HD11	1:B:177:ILE:HB	1.81	0.61
1:F:66:LEU:C	1:F:66:LEU:HD12	2.24	0.61
1:I:120:LEU:HD11	1:I:127:ALA:HB2	1.82	0.61
1:F:177:ILE:H	1:F:178:PRO:HA	1.66	0.61
1:H:158:VAL:O	1:H:162:LEU:CB	2.44	0.61
1:I:69:GLU:O	1:I:70:GLY:C	2.43	0.61
1:I:138:LEU:HD13	1:J:138:LEU:HD21	1.74	0.61
1:J:84:PHE:O	1:J:85:ALA:HB3	2.00	0.60
1:C:123:ASN:N	1:C:123:ASN:HD22	1.99	0.60
1:G:11:LEU:O	1:G:17:PHE:HB2	2.00	0.60
1:A:153:ALA:O	1:A:157:VAL:HG23	2.00	0.60
1:G:153:ALA:O	1:G:157:VAL:HG23	2.02	0.60
1:J:156:ARG:HB2	1:J:191:GLN:NE2	2.16	0.60
1:J:108:LEU:HD12	1:J:108:LEU:N	2.15	0.60
1:J:151:LYS:O	1:J:155:HIS:CD2	2.54	0.60
1:A:36:ASN:OD1	1:A:107:GLN:HG3	2.02	0.60
1:A:124:THR:N	1:A:125:PRO:CD	2.63	0.60
1:E:52:ALA:HB1	1:E:111:PHE:O	2.01	0.60
1:H:141:ARG:O	1:H:145:ILE:HG13	2.00	0.60
1:I:159:ARG:NE	1:J:159:ARG:HD2	2.16	0.60
1:D:124:THR:HG1	1:D:125:PRO:HD3	1.63	0.60
1:D:188:LEU:O	1:D:189:SER:C	2.45	0.60
1:J:138:LEU:O	1:J:142:ILE:HG13	2.02	0.60
1:H:174:ARG:O	1:H:175:VAL:CB	2.47	0.60
1:A:15:HIS:CE1	1:A:16:LEU:HG	2.37	0.60
1:G:67:THR:HB	1:G:68:PRO:HD2	1.82	0.60
1:J:57:ILE:HD11	1:J:109:PHE:CE1	2.37	0.60
1:F:215:ILE:N	1:F:215:ILE:CD1	2.65	0.59
1:C:34:LEU:O	1:C:35:VAL:HB	2.02	0.59
1:D:123:ASN:ND2	1:D:125:PRO:HD2	2.17	0.59
1:E:88:MET:HE3	1:E:93:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:VAL:HG11	1:C:198:ILE:HG21	1.84	0.59
1:E:21:SER:C	1:E:23:VAL:H	2.10	0.59
1:I:29:LEU:HD23	1:I:111:PHE:HE2	1.68	0.59
1:A:57:ILE:HD11	1:A:109:PHE:HD1	1.67	0.59
1:G:15:HIS:CE1	1:G:16:LEU:HG	2.38	0.59
1:I:156:ARG:HB2	1:I:188:LEU:HD22	1.82	0.59
1:B:108:LEU:HD12	1:B:108:LEU:N	2.17	0.59
1:J:197:ARG:O	1:J:201:ARG:HG3	2.03	0.59
1:D:75:LEU:N	1:D:75:LEU:HD12	2.17	0.59
1:B:124:THR:H	1:B:125:PRO:HD3	1.67	0.59
1:B:150:LEU:O	1:B:154:THR:HG23	2.03	0.59
1:C:68:PRO:O	1:C:69:GLU:HB2	2.03	0.59
1:J:190:ILE:O	1:J:190:ILE:HG22	2.01	0.59
1:D:108:LEU:HD12	1:D:108:LEU:C	2.28	0.59
1:E:68:PRO:HG2	1:E:69:GLU:OE1	2.03	0.59
1:D:89:MET:CA	1:D:89:MET:CE	2.78	0.58
1:J:34:LEU:HD11	1:J:107:GLN:HE21	1.67	0.58
1:E:107:GLN:HE22	1:H:6:VAL:HG22	1.67	0.58
1:A:19:PRO:HG2	1:A:130:LEU:HD23	1.85	0.58
1:A:67:THR:HB	1:A:68:PRO:HD2	1.85	0.58
1:B:124:THR:H	1:B:125:PRO:CD	2.16	0.58
1:A:81:ARG:O	1:A:82:ASN:OD1	2.21	0.58
1:E:57:ILE:O	1:H:9:GLN:NE2	2.36	0.58
1:D:89:MET:HE2	1:D:89:MET:O	2.03	0.58
1:G:79:ASN:CG	1:G:80:GLU:H	2.10	0.58
1:C:207:ILE:C	1:C:208:ILE:HG23	2.29	0.58
1:J:62:LYS:HZ2	1:J:101:GLN:HB3	1.68	0.58
1:J:179:VAL:O	1:J:179:VAL:HG12	2.04	0.58
1:D:148:LEU:HD12	1:D:148:LEU:C	2.27	0.57
1:E:21:SER:C	1:E:23:VAL:N	2.59	0.57
1:E:21:SER:HB3	1:G:191:GLN:CD	2.29	0.57
1:J:141:ARG:O	1:J:145:ILE:HG13	2.04	0.57
1:A:57:ILE:N	1:A:57:ILE:CD1	2.67	0.57
1:G:14:HIS:O	1:G:18:GLU:HG3	2.04	0.57
1:B:123:ASN:ND2	1:B:126:LEU:CB	2.66	0.57
1:J:1:MET:SD	1:J:1:MET:N	2.77	0.57
1:D:84:PHE:O	1:D:85:ALA:HB3	2.03	0.57
1:C:124:THR:C	1:C:126:LEU:H	2.13	0.57
1:G:210:LEU:HD11	1:G:215:ILE:HD12	1.87	0.57
1:C:208:ILE:HD12	1:C:208:ILE:O	2.05	0.57
1:G:190:ILE:CG2	1:G:192:PRO:CD	2.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:CD1	1:A:3:PHE:N	2.73	0.57
1:D:4:GLN:HB2	1:D:7:HIS:HD2	1.70	0.57
1:F:153:ALA:O	1:F:157:VAL:HG23	2.05	0.57
1:G:49:PRO:HA	1:G:95:ASN:HD22	1.68	0.57
1:I:139:HIS:CE1	1:J:86:GLU:OE2	2.58	0.57
1:J:130:LEU:HD23	1:J:130:LEU:C	2.30	0.57
1:A:128:LEU:HD21	1:B:90:PHE:C	2.29	0.56
1:D:74:ILE:C	1:D:75:LEU:HD12	2.30	0.56
1:G:70:GLY:O	1:G:71:GLN:HB2	2.04	0.56
1:J:124:THR:CB	1:J:125:PRO:HD3	2.32	0.56
1:B:217:ILE:HD13	1:B:223:LEU:HD11	1.86	0.56
1:E:156:ARG:O	1:E:188:LEU:HD13	2.06	0.56
1:I:50:ALA:HA	1:I:96:TYR:CE2	2.41	0.56
1:A:213:ARG:HH12	1:H:30:ALA:HA	1.66	0.56
1:I:123:ASN:HD22	1:I:126:LEU:HD12	1.70	0.56
1:I:138:LEU:HB2	1:J:138:LEU:HD21	1.86	0.56
1:H:89:MET:HE2	1:H:113:ASN:HA	1.88	0.56
1:A:124:THR:O	1:A:126:LEU:N	2.39	0.56
1:A:133:LYS:HA	1:A:136:THR:HG22	1.88	0.56
1:G:132:ALA:O	1:G:136:THR:HG23	2.06	0.56
1:F:66:LEU:O	1:F:66:LEU:CD1	2.53	0.56
1:G:124:THR:N	1:G:125:PRO:CD	2.69	0.56
1:I:67:THR:OG1	1:I:68:PRO:HD2	2.06	0.56
1:B:63:ILE:O	1:B:64:TYR:CD1	2.59	0.55
1:D:63:ILE:O	1:D:64:TYR:CD1	2.60	0.55
1:G:18:GLU:N	1:G:19:PRO:CD	2.69	0.55
1:B:119:GLN:O	1:B:126:LEU:HD23	2.07	0.55
1:H:154:THR:O	1:H:158:VAL:HG23	2.06	0.55
1:F:18:GLU:HB3	1:F:19:PRO:HD3	1.88	0.55
1:A:63:ILE:O	1:A:64:TYR:O	2.24	0.55
1:H:217:ILE:HG22	1:H:218:LEU:HG	1.87	0.55
1:H:138:LEU:O	1:H:142:ILE:HG13	2.06	0.55
1:A:140:GLN:O	1:A:144:GLU:HG3	2.06	0.55
1:B:124:THR:CG2	1:B:125:PRO:CD	2.84	0.55
1:H:214:GLU:N	1:H:214:GLU:OE1	2.40	0.55
1:I:8:GLN:HE22	1:I:25:LEU:HD13	1.70	0.55
1:I:140:GLN:O	1:I:144:GLU:HG3	2.06	0.55
1:A:84:PHE:O	1:A:85:ALA:HB3	2.06	0.55
1:F:150:LEU:O	1:F:154:THR:HG23	2.06	0.55
1:F:202:LEU:HD23	1:F:202:LEU:C	2.29	0.55
1:G:151:LYS:O	1:G:155:HIS:CD2	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:175:VAL:HG12	1:H:176:GLU:N	2.21	0.55
1:C:39:LYS:HB3	1:C:105:PRO:HD3	1.89	0.55
1:H:144:GLU:HA	1:H:147:THR:HG22	1.88	0.55
1:C:131:LEU:CD2	1:D:131:LEU:HD21	2.36	0.54
1:H:140:GLN:O	1:H:144:GLU:HG3	2.07	0.54
1:C:202:LEU:C	1:C:202:LEU:HD12	2.32	0.54
1:E:123:ASN:O	1:E:124:THR:C	2.50	0.54
1:F:177:ILE:HB	1:F:178:PRO:C	2.32	0.54
1:G:57:ILE:HD11	1:G:109:PHE:HD1	1.72	0.54
1:H:89:MET:HG2	1:H:117:LEU:HD21	1.89	0.54
1:I:124:THR:HG22	1:I:125:PRO:HD3	1.89	0.54
1:I:188:LEU:C	1:I:189:SER:HG	2.08	0.54
1:D:18:GLU:H	1:D:19:PRO:HD2	1.73	0.54
1:E:152:ASN:CG	1:F:152:ASN:ND2	2.66	0.54
1:A:4:GLN:O	1:A:5:ARG:CB	2.56	0.54
1:E:45:ARG:HA	1:E:99:THR:HG23	1.88	0.54
1:J:18:GLU:N	1:J:19:PRO:HD2	2.23	0.54
1:A:8:GLN:HG3	1:A:25:LEU:HD23	1.90	0.54
1:H:45:ARG:HA	1:H:99:THR:HG23	1.88	0.54
1:I:131:LEU:CD2	1:J:131:LEU:HD21	2.36	0.54
1:J:196:SER:O	1:J:200:HIS:CD2	2.61	0.54
1:A:123:ASN:C	1:A:125:PRO:CD	2.78	0.53
1:D:15:HIS:CE1	1:D:16:LEU:HG	2.43	0.53
1:F:108:LEU:N	1:F:108:LEU:CD1	2.70	0.53
1:J:43:VAL:HG12	1:J:44:PHE:HD1	1.73	0.53
1:H:108:LEU:N	1:H:108:LEU:CD1	2.71	0.53
1:J:57:ILE:HD11	1:J:109:PHE:CD1	2.43	0.53
1:D:176:GLU:O	1:D:177:ILE:C	2.52	0.53
1:A:141:ARG:O	1:A:145:ILE:HG13	2.09	0.53
1:C:65:ARG:O	1:C:65:ARG:HD3	2.09	0.53
1:I:8:GLN:HE22	1:I:25:LEU:HB3	1.73	0.53
1:I:43:VAL:HG12	1:I:44:PHE:HD1	1.73	0.53
1:B:50:ALA:HA	1:B:96:TYR:CE2	2.44	0.53
1:E:6:VAL:CG1	1:H:7:HIS:HE1	2.17	0.53
1:E:119:GLN:H	1:E:119:GLN:NE2	2.07	0.53
1:E:188:LEU:O	1:E:189:SER:OG	2.21	0.53
1:G:57:ILE:HD11	1:G:109:PHE:CD1	2.44	0.53
1:D:64:TYR:HA	1:D:74:ILE:HA	1.91	0.53
1:H:57:ILE:N	1:H:57:ILE:CD1	2.65	0.53
1:H:122:ASP:O	1:H:123:ASN:HB2	2.09	0.53
1:C:212:GLY:O	1:C:214:GLU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:GLU:N	1:H:19:PRO:CD	2.72	0.53
1:E:14:HIS:HD2	1:E:16:LEU:H	1.56	0.52
1:H:167:HIS:HB3	1:H:219:ASP:HB2	1.92	0.52
1:F:18:GLU:N	1:F:19:PRO:CD	2.71	0.52
1:F:63:ILE:O	1:F:64:TYR:O	2.27	0.52
1:B:59:GLY:HA3	1:B:106:SER:OG	2.09	0.52
1:C:210:LEU:HD12	1:C:210:LEU:N	2.17	0.52
1:H:175:VAL:CG1	1:H:176:GLU:N	2.72	0.52
1:I:3:PHE:O	1:I:4:GLN:HB2	2.10	0.52
1:E:217:ILE:HG12	1:E:218:LEU:N	2.25	0.52
1:F:75:LEU:HD12	1:F:75:LEU:N	2.25	0.52
1:J:195:PHE:O	1:J:199:MET:HG2	2.10	0.52
1:C:50:ALA:HA	1:C:96:TYR:CZ	2.45	0.52
1:F:66:LEU:C	1:F:66:LEU:CD1	2.82	0.52
1:G:75:LEU:N	1:G:75:LEU:HD12	2.24	0.52
1:A:88:MET:HE3	1:A:93:THR:HG1	1.74	0.52
1:C:19:PRO:CG	1:C:130:LEU:HD23	2.33	0.52
1:C:38:ASP:OD1	1:C:39:LYS:N	2.36	0.52
1:D:15:HIS:HB3	1:D:137:ARG:CD	2.40	0.52
1:B:124:THR:HG23	1:B:125:PRO:HD3	1.90	0.52
1:J:156:ARG:HB2	1:J:191:GLN:HE22	1.73	0.52
1:C:108:LEU:N	1:C:108:LEU:CD1	2.72	0.51
1:D:20:LEU:H	1:D:20:LEU:CD1	2.22	0.51
1:E:14:HIS:CD2	1:E:16:LEU:H	2.28	0.51
1:E:120:LEU:HD23	1:F:128:LEU:HD21	1.92	0.51
1:A:207:ILE:HG21	1:A:223:LEU:HD21	1.92	0.51
1:B:217:ILE:HD13	1:B:223:LEU:CD1	2.39	0.51
1:F:44:PHE:HE1	1:F:84:PHE:HE2	1.58	0.51
1:G:84:PHE:O	1:G:85:ALA:HB3	2.09	0.51
1:J:227:GLU:C	1:J:227:GLU:CD	2.78	0.51
1:D:51:HIS:O	1:D:52:ALA:HB3	2.11	0.51
1:G:50:ALA:HA	1:G:96:TYR:CE2	2.45	0.51
1:H:65:ARG:O	1:H:66:LEU:HB2	2.09	0.51
1:B:91:MET:O	1:B:92:ASP:C	2.51	0.51
1:C:4:GLN:HB2	1:C:7:HIS:HD2	1.74	0.51
1:E:67:THR:HB	1:E:68:PRO:HD2	1.91	0.51
1:J:174:ARG:O	1:J:175:VAL:CB	2.57	0.51
1:B:57:ILE:HD11	1:B:109:PHE:HD1	1.76	0.51
1:C:10:LEU:HD21	1:I:10:LEU:HG	1.93	0.51
1:C:88:MET:HE1	1:C:97:VAL:HG22	1.93	0.51
1:J:123:ASN:C	1:J:125:PRO:HD2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:THR:N	1:G:125:PRO:HD2	2.25	0.51
1:A:108:LEU:N	1:A:108:LEU:CD1	2.73	0.51
1:A:177:ILE:C	1:A:179:VAL:H	2.19	0.51
1:C:33:ASP:OD1	1:C:34:LEU:N	2.43	0.51
1:D:63:ILE:O	1:D:64:TYR:O	2.29	0.51
1:D:20:LEU:HD12	1:D:20:LEU:H	1.76	0.51
1:D:89:MET:CE	1:D:89:MET:O	2.59	0.51
1:G:132:ALA:HB2	1:H:90:PHE:HB2	1.93	0.51
1:H:20:LEU:HD23	1:H:126:LEU:HD11	1.92	0.51
1:I:69:GLU:OE1	1:I:69:GLU:C	2.53	0.51
1:I:131:LEU:HD22	1:J:130:LEU:HD22	1.92	0.51
1:I:150:LEU:O	1:I:154:THR:HG23	2.11	0.51
1:A:202:LEU:HD13	1:A:208:ILE:HD12	1.93	0.51
1:C:11:LEU:O	1:C:17:PHE:HB2	2.11	0.51
1:D:124:THR:OG1	1:D:125:PRO:CD	2.41	0.51
1:A:124:THR:C	1:A:126:LEU:N	2.69	0.50
1:F:143:ASP:O	1:F:147:THR:HG23	2.10	0.50
1:F:214:GLU:C	1:F:215:ILE:HD12	2.34	0.50
1:J:123:ASN:C	1:J:124:THR:OG1	2.51	0.50
1:C:10:LEU:HD23	1:I:10:LEU:HD21	1.89	0.50
1:J:19:PRO:HD3	1:J:133:LYS:HG3	1.93	0.50
1:D:97:VAL:O	1:D:97:VAL:HG22	2.10	0.50
1:G:190:ILE:HG22	1:G:191:GLN:N	2.26	0.50
1:H:75:LEU:HD12	1:H:75:LEU:N	2.26	0.50
1:I:18:GLU:N	1:I:19:PRO:CD	2.74	0.50
1:C:131:LEU:HG	1:D:131:LEU:HD21	1.93	0.50
1:C:141:ARG:O	1:C:145:ILE:HG13	2.11	0.50
1:C:29:LEU:HD23	1:C:111:PHE:HE2	1.76	0.50
1:J:18:GLU:N	1:J:19:PRO:CD	2.75	0.50
1:E:25:LEU:N	1:E:25:LEU:HD12	2.26	0.50
1:F:124:THR:H	1:F:125:PRO:HD3	1.77	0.50
1:B:56:LEU:C	1:B:57:ILE:HD12	2.36	0.50
1:C:124:THR:C	1:C:126:LEU:N	2.68	0.50
1:D:144:GLU:O	1:D:148:LEU:HG	2.12	0.50
1:G:202:LEU:HD21	1:G:209:HIS:HB2	1.93	0.50
1:J:75:LEU:N	1:J:75:LEU:CD1	2.75	0.50
1:G:151:LYS:O	1:G:155:HIS:HD2	1.93	0.50
1:H:88:MET:HA	1:H:91:MET:HB2	1.94	0.50
1:I:3:PHE:HB2	1:I:4:GLN:OE1	2.12	0.50
1:I:84:PHE:O	1:I:85:ALA:HB3	2.11	0.50
1:J:7:HIS:HA	1:J:10:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:CG	1:B:131:LEU:HD21	2.42	0.49
1:D:91:MET:O	1:D:92:ASP:HB2	2.12	0.49
1:H:63:ILE:O	1:H:64:TYR:O	2.30	0.49
1:H:123:ASN:C	1:H:125:PRO:CD	2.78	0.49
1:H:189:SER:OG	1:H:194:THR:HG23	2.12	0.49
1:I:155:HIS:CA	1:I:159:ARG:NH1	2.75	0.49
1:A:172:ASN:HB2	1:A:217:ILE:HB	1.94	0.49
1:F:177:ILE:HG21	1:F:179:VAL:O	2.12	0.49
1:G:67:THR:CB	1:G:68:PRO:HD2	2.42	0.49
1:A:164:LEU:C	1:A:164:LEU:CD1	2.84	0.49
1:G:63:ILE:HG22	1:G:98:ALA:HB1	1.93	0.49
1:D:15:HIS:HB3	1:D:137:ARG:HD2	1.94	0.49
1:D:108:LEU:C	1:D:108:LEU:CD1	2.86	0.49
1:G:140:GLN:O	1:G:144:GLU:HG2	2.13	0.49
1:A:212:GLY:O	1:A:213:ARG:HB3	2.13	0.49
1:B:50:ALA:H	1:B:95:ASN:HA	1.76	0.49
1:F:202:LEU:CD2	1:F:202:LEU:C	2.85	0.49
1:J:150:LEU:O	1:J:154:THR:HG23	2.12	0.49
1:B:124:THR:HG23	1:B:125:PRO:CD	2.42	0.49
1:A:185:ALA:HB1	1:A:190:ILE:HD11	1.95	0.49
1:A:212:GLY:C	1:A:214:GLU:H	2.21	0.49
1:J:221:GLU:N	1:J:221:GLU:OE1	2.45	0.49
1:C:124:THR:HB	1:C:125:PRO:CD	2.41	0.49
1:F:63:ILE:O	1:F:64:TYR:CG	2.66	0.49
1:B:158:VAL:HG12	1:B:158:VAL:O	2.13	0.49
1:I:15:HIS:CE1	1:I:16:LEU:HG	2.47	0.49
1:A:49:PRO:HA	1:A:95:ASN:OD1	2.13	0.49
1:C:59:GLY:HA3	1:C:106:SER:OG	2.12	0.49
1:C:157:VAL:HG13	1:C:158:VAL:N	2.28	0.49
1:G:57:ILE:HD12	1:G:57:ILE:H	1.75	0.49
1:C:57:ILE:HD13	1:C:107:GLN:O	2.13	0.48
1:I:124:THR:HG23	1:I:125:PRO:HD3	1.95	0.48
1:J:130:LEU:O	1:J:130:LEU:CD2	2.51	0.48
1:A:50:ALA:HA	1:A:96:TYR:CE2	2.49	0.48
1:G:144:GLU:OE2	1:H:145:ILE:CG1	2.61	0.48
1:G:164:LEU:HD13	1:G:172:ASN:HB3	1.95	0.48
1:I:19:PRO:HG3	1:I:130:LEU:HD23	1.94	0.48
1:J:172:ASN:O	1:J:173:CYS:C	2.57	0.48
1:G:131:LEU:HD22	1:H:130:LEU:HD22	1.96	0.48
1:A:34:LEU:HD11	1:A:107:GLN:NE2	2.28	0.48
1:A:124:THR:O	1:A:125:PRO:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:PRO:O	1:D:69:GLU:C	2.56	0.48
1:I:151:LYS:O	1:I:155:HIS:CD2	2.66	0.48
1:A:154:THR:HA	1:A:198:ILE:HD13	1.94	0.48
1:C:91:MET:O	1:C:93:THR:HG23	2.13	0.48
1:B:44:PHE:H	1:B:100:ALA:HB3	1.79	0.48
1:D:93:THR:H	1:D:94:PRO:HD3	1.75	0.48
1:D:93:THR:N	1:D:94:PRO:CD	2.76	0.48
1:E:52:ALA:CB	1:E:112:SER:HA	2.44	0.48
1:A:188:LEU:O	1:A:189:SER:OG	2.30	0.48
1:B:213:ARG:O	1:B:214:GLU:O	2.31	0.48
1:B:188:LEU:O	1:B:189:SER:OG	2.28	0.47
1:G:19:PRO:HG3	1:G:133:LYS:HG3	1.95	0.47
1:G:68:PRO:O	1:G:69:GLU:HB2	2.13	0.47
1:A:167:HIS:O	1:A:168:ALA:CB	2.62	0.47
1:C:212:GLY:O	1:C:213:ARG:C	2.57	0.47
1:C:208:ILE:CD1	1:C:209:HIS:N	2.77	0.47
1:C:6:VAL:HG22	1:I:57:ILE:HD13	1.97	0.47
1:J:151:LYS:O	1:J:155:HIS:HD2	1.96	0.47
1:C:43:VAL:HG12	1:C:44:PHE:HD1	1.80	0.47
1:G:18:GLU:HB2	1:G:19:PRO:HD3	1.96	0.47
1:H:204:ASP:O	1:H:205:GLU:HB2	2.14	0.47
1:J:3:PHE:HE2	1:J:34:LEU:HD22	1.79	0.47
1:C:213:ARG:O	1:C:214:GLU:HB2	2.15	0.47
1:D:20:LEU:N	1:D:20:LEU:CD1	2.76	0.47
1:F:44:PHE:H	1:F:100:ALA:HB3	1.80	0.47
1:F:66:LEU:O	1:F:66:LEU:HD13	2.14	0.47
1:H:80:GLU:O	1:H:81:ARG:HB2	2.15	0.47
1:I:86:GLU:OE1	1:I:86:GLU:N	2.38	0.47
1:C:210:LEU:CD1	1:C:210:LEU:N	2.77	0.47
1:D:75:LEU:N	1:D:75:LEU:CD1	2.78	0.47
1:G:63:ILE:O	1:G:64:TYR:CG	2.68	0.47
1:D:73:LYS:HD2	1:D:75:LEU:HD11	1.97	0.47
1:J:108:LEU:N	1:J:108:LEU:CD1	2.78	0.47
1:C:124:THR:O	1:C:126:LEU:N	2.47	0.46
1:E:15:HIS:ND1	1:E:16:LEU:HG	2.30	0.46
1:G:20:LEU:HD21	1:G:119:GLN:CD	2.40	0.46
1:G:40:GLY:HA2	1:G:101:GLN:NE2	2.27	0.46
1:G:94:PRO:O	1:G:95:ASN:ND2	2.47	0.46
1:F:135:SER:O	1:F:139:HIS:HD2	1.97	0.46
1:F:177:ILE:HB	1:F:178:PRO:CA	2.45	0.46
1:G:18:GLU:OE1	1:G:133:LYS:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:SER:O	1:H:139:HIS:HD2	1.98	0.46
1:J:123:ASN:O	1:J:125:PRO:HD3	2.15	0.46
1:G:117:LEU:O	1:G:121:GLN:HG3	2.16	0.46
1:J:88:MET:CE	1:J:93:THR:OG1	2.63	0.46
1:A:135:SER:O	1:A:139:HIS:CD2	2.69	0.46
1:B:18:GLU:N	1:B:19:PRO:CD	2.79	0.46
1:G:1:MET:O	1:G:2:GLU:HB2	2.16	0.46
1:I:127:ALA:O	1:I:131:LEU:HG	2.15	0.46
1:A:207:ILE:HG21	1:A:223:LEU:CD2	2.46	0.46
1:I:80:GLU:H	1:I:80:GLU:CD	2.22	0.46
1:A:64:TYR:CB	1:A:74:ILE:HD13	2.43	0.46
1:F:16:LEU:HD11	1:F:86:GLU:OE1	2.16	0.46
1:G:196:SER:O	1:G:200:HIS:ND1	2.49	0.46
1:E:116:TYR:HA	1:E:119:GLN:HE22	1.80	0.46
1:I:56:LEU:HD13	1:I:108:LEU:HD21	1.98	0.46
1:J:6:VAL:HG22	1:J:6:VAL:O	2.14	0.46
1:I:59:GLY:HA3	1:I:106:SER:OG	2.16	0.46
1:J:81:ARG:O	1:J:82:ASN:OD1	2.34	0.46
1:J:88:MET:HE1	1:J:93:THR:OG1	2.16	0.46
1:A:124:THR:O	1:A:127:ALA:N	2.49	0.45
1:H:123:ASN:CA	1:H:125:PRO:HD2	2.46	0.45
1:D:67:THR:O	1:D:68:PRO:C	2.58	0.45
1:H:84:PHE:O	1:H:85:ALA:HB3	2.15	0.45
1:J:132:ALA:O	1:J:136:THR:HG23	2.16	0.45
1:A:190:ILE:HD13	1:A:191:GLN:O	2.16	0.45
1:F:177:ILE:N	1:F:178:PRO:CA	2.78	0.45
1:G:216:SER:OG	1:G:219:ASP:OD1	2.34	0.45
1:A:138:LEU:O	1:A:142:ILE:HG13	2.15	0.45
1:D:18:GLU:N	1:D:19:PRO:CD	2.77	0.45
1:D:89:MET:CE	1:D:89:MET:C	2.90	0.45
1:F:47:GLY:HA2	1:H:224:GLU:HG2	1.97	0.45
1:H:63:ILE:O	1:H:64:TYR:CD1	2.69	0.45
1:H:120:LEU:O	1:H:121:GLN:C	2.59	0.45
1:A:131:LEU:HD21	1:B:131:LEU:CG	2.47	0.45
1:H:158:VAL:HG21	1:H:225:CYS:HB3	1.98	0.45
1:J:15:HIS:CE1	1:J:16:LEU:HG	2.52	0.45
1:J:18:GLU:HB2	1:J:19:PRO:HD3	1.98	0.45
1:B:99:THR:CG2	1:B:100:ALA:N	2.63	0.45
1:E:159:ARG:O	1:E:163:THR:HG23	2.16	0.45
1:E:184:VAL:HG21	1:E:195:PHE:CZ	2.51	0.45
1:C:92:ASP:O	1:C:93:THR:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:ILE:O	1:H:64:TYR:CG	2.70	0.45
1:J:213:ARG:O	1:J:215:ILE:N	2.42	0.45
1:H:25:LEU:O	1:H:29:LEU:HG	2.17	0.45
1:D:104:VAL:O	1:D:105:PRO:C	2.59	0.45
1:D:148:LEU:C	1:D:148:LEU:CD1	2.90	0.45
1:H:57:ILE:HD11	1:H:109:PHE:HD1	1.82	0.45
1:I:124:THR:CG2	1:I:125:PRO:CD	2.95	0.45
1:A:43:VAL:HG12	1:A:44:PHE:HD1	1.81	0.44
1:B:84:PHE:O	1:B:85:ALA:HB3	2.15	0.44
1:E:15:HIS:CE1	1:E:16:LEU:HG	2.52	0.44
1:F:11:LEU:HD22	1:F:11:LEU:N	2.32	0.44
1:I:93:THR:HA	1:I:94:PRO:HD3	1.87	0.44
1:C:212:GLY:C	1:C:214:GLU:N	2.75	0.44
1:A:18:GLU:N	1:A:19:PRO:CD	2.80	0.44
1:C:63:ILE:HD11	1:C:84:PHE:CD2	2.52	0.44
1:E:21:SER:O	1:E:22:PRO:C	2.59	0.44
1:G:137:ARG:HB2	1:H:138:LEU:HD13	1.99	0.44
1:H:177:ILE:HA	1:H:178:PRO:HD3	1.85	0.44
1:J:34:LEU:HD11	1:J:107:GLN:NE2	2.30	0.44
1:B:22:PRO:O	1:B:26:GLN:HG2	2.17	0.44
1:C:61:VAL:HG22	1:C:102:ALA:HB2	2.00	0.44
1:H:43:VAL:HG12	1:H:44:PHE:HD1	1.81	0.44
1:I:90:PHE:HD2	1:J:128:LEU:HB3	1.83	0.44
1:I:155:HIS:HB3	1:I:159:ARG:NH1	2.32	0.44
1:J:183:LEU:HD22	1:J:193:GLU:HB3	2.00	0.44
1:C:90:PHE:HB3	1:D:128:LEU:HB3	1.99	0.44
1:D:103:VAL:O	1:D:103:VAL:HG23	2.17	0.44
1:B:108:LEU:N	1:B:108:LEU:CD1	2.80	0.44
1:C:87:ALA:O	1:C:91:MET:HB2	2.18	0.44
1:J:123:ASN:C	1:J:125:PRO:CD	2.91	0.44
1:A:67:THR:CB	1:A:68:PRO:HD2	2.48	0.44
1:C:202:LEU:C	1:C:202:LEU:CD1	2.90	0.44
1:E:55:TYR:CE1	1:E:57:ILE:HD13	2.52	0.44
1:B:57:ILE:HD12	1:B:57:ILE:H	1.79	0.43
1:D:79:ASN:ND2	1:D:80:GLU:H	2.16	0.43
1:G:3:PHE:O	1:G:4:GLN:HB2	2.18	0.43
1:C:89:MET:HE3	1:C:90:PHE:CE2	2.53	0.43
1:E:23:VAL:O	1:E:24:GLN:C	2.59	0.43
1:G:137:ARG:CB	1:H:138:LEU:HD13	2.47	0.43
1:J:144:GLU:O	1:J:148:LEU:HG	2.19	0.43
1:C:57:ILE:HD11	1:C:109:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ILE:C	1:C:208:ILE:CG2	2.90	0.43
1:E:124:THR:CB	1:E:125:PRO:HD3	2.20	0.43
1:I:67:THR:O	1:I:68:PRO:C	2.61	0.43
1:C:67:THR:HG22	1:C:68:PRO:N	2.33	0.43
1:E:139:HIS:HE1	1:F:86:GLU:HG2	1.83	0.43
1:E:212:GLY:O	1:E:213:ARG:CB	2.63	0.43
1:G:79:ASN:H	1:G:82:ASN:HD21	1.66	0.43
1:G:121:GLN:O	1:G:122:ASP:CB	2.65	0.43
1:J:57:ILE:HD11	1:J:109:PHE:HE1	1.83	0.43
1:D:123:ASN:HD22	1:D:123:ASN:C	2.26	0.43
1:E:49:PRO:HA	1:E:95:ASN:HD22	1.84	0.43
1:G:143:ASP:O	1:G:147:THR:HG23	2.18	0.43
1:H:95:ASN:N	1:H:95:ASN:ND2	2.64	0.43
1:C:45:ARG:HA	1:C:99:THR:HG23	2.00	0.43
1:D:67:THR:OG1	1:D:68:PRO:HD2	2.18	0.43
1:E:18:GLU:N	1:E:19:PRO:CD	2.81	0.43
1:I:80:GLU:OE1	1:I:80:GLU:N	2.41	0.43
1:A:3:PHE:HB2	1:A:4:GLN:H	1.53	0.43
1:A:88:MET:HE3	1:A:93:THR:CB	2.49	0.43
1:D:11:LEU:HD23	1:D:55:TYR:CZ	2.54	0.43
1:H:130:LEU:HD23	1:H:130:LEU:C	2.38	0.43
1:I:19:PRO:CG	1:I:130:LEU:HD23	2.49	0.43
1:A:14:HIS:HB3	1:A:17:PHE:HD1	1.84	0.43
1:A:131:LEU:HG	1:B:131:LEU:HD21	2.00	0.43
1:B:225:CYS:O	1:B:226:PHE:C	2.61	0.43
1:C:57:ILE:HD12	1:C:57:ILE:H	1.79	0.43
1:F:63:ILE:HG23	1:F:99:THR:O	2.19	0.43
1:I:8:GLN:NE2	1:I:25:LEU:CD1	2.78	0.43
1:J:130:LEU:C	1:J:130:LEU:CD2	2.91	0.43
1:A:138:LEU:HD21	1:A:142:ILE:HD11	2.00	0.42
1:B:151:LYS:O	1:B:155:HIS:ND1	2.52	0.42
1:C:15:HIS:CE1	1:C:16:LEU:HG	2.55	0.42
1:C:38:ASP:OD1	1:C:105:PRO:HG3	2.18	0.42
1:D:73:LYS:HA	1:J:74:ILE:HB	2.01	0.42
1:C:65:ARG:O	1:C:66:LEU:HB2	2.18	0.42
1:A:207:ILE:CG2	1:A:223:LEU:HD21	2.49	0.42
1:H:86:GLU:CD	1:H:86:GLU:H	2.26	0.42
1:I:86:GLU:OE2	1:J:139:HIS:CE1	2.72	0.42
1:J:134:LEU:O	1:J:138:LEU:HG	2.17	0.42
1:D:148:LEU:HD12	1:D:149:SER:H	1.78	0.42
1:H:175:VAL:O	1:H:176:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:ARG:NH2	1:J:159:ARG:HD2	2.33	0.42
1:A:61:VAL:HG21	1:A:108:LEU:HD21	2.02	0.42
1:C:18:GLU:CB	1:C:19:PRO:HD3	2.27	0.42
1:C:159:ARG:O	1:C:163:THR:HG23	2.18	0.42
1:H:214:GLU:N	1:H:214:GLU:CD	2.77	0.42
1:A:187:HIS:HD2	1:C:91:MET:HA	1.84	0.42
1:B:55:TYR:CE1	1:B:57:ILE:HG13	2.54	0.42
1:C:206:GLY:O	1:C:219:ASP:OD2	2.37	0.42
1:D:50:ALA:HA	1:D:96:TYR:CE2	2.55	0.42
1:J:28:LEU:HB2	1:J:119:GLN:HE22	1.84	0.42
1:C:220:ARG:O	1:C:221:GLU:HB2	2.20	0.42
1:B:15:HIS:CE1	1:B:16:LEU:HG	2.55	0.42
1:E:21:SER:HB3	1:G:191:GLN:OE1	2.20	0.42
1:F:15:HIS:CE1	1:F:16:LEU:HG	2.54	0.42
1:H:21:SER:HB2	1:H:22:PRO:HD2	2.01	0.42
1:J:37:LEU:HB3	1:J:41:ALA:HB3	2.02	0.42
1:A:91:MET:O	1:A:92:ASP:HB2	2.20	0.42
1:A:103:VAL:HG23	1:A:104:VAL:HG13	2.02	0.42
1:C:29:LEU:HD23	1:C:111:PHE:CE2	2.54	0.42
1:C:157:VAL:O	1:C:161:LEU:HG	2.20	0.42
1:I:155:HIS:HA	1:I:159:ARG:HH12	1.84	0.42
1:J:63:ILE:HD11	1:J:84:PHE:CD2	2.55	0.42
1:B:55:TYR:HD2	1:B:83:THR:HG22	1.85	0.41
1:E:88:MET:HE1	1:E:93:THR:HG21	2.02	0.41
1:G:75:LEU:N	1:G:75:LEU:CD1	2.83	0.41
1:G:88:MET:HE3	1:G:93:THR:CB	2.50	0.41
1:H:75:LEU:N	1:H:75:LEU:CD1	2.83	0.41
1:J:223:LEU:O	1:J:227:GLU:HB3	2.20	0.41
1:B:25:LEU:O	1:B:29:LEU:HG	2.20	0.41
1:A:11:LEU:O	1:A:17:PHE:HB2	2.21	0.41
1:C:19:PRO:HG2	1:C:130:LEU:CD2	2.38	0.41
1:E:69:GLU:OE1	1:E:69:GLU:N	2.50	0.41
1:G:11:LEU:HB3	1:G:17:PHE:CG	2.56	0.41
1:I:180:ALA:HB3	1:I:183:LEU:HG	2.03	0.41
1:I:204:ASP:OD1	1:I:205:GLU:N	2.53	0.41
1:C:10:LEU:HD21	1:I:10:LEU:CD2	2.49	0.41
1:E:21:SER:CA	1:G:191:GLN:OE1	2.69	0.41
1:E:152:ASN:CG	1:F:152:ASN:HD21	2.28	0.41
1:I:154:THR:HA	1:I:198:ILE:HD13	2.02	0.41
1:B:55:TYR:HD2	1:B:83:THR:CG2	2.32	0.41
1:F:8:GLN:O	1:F:12:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:PRO:HB2	1:I:51:HIS:CD2	2.56	0.41
1:I:141:ARG:O	1:I:145:ILE:HG13	2.20	0.41
1:A:178:PRO:HG2	1:H:3:PHE:H	1.85	0.41
1:E:10:LEU:HD13	1:H:10:LEU:HD13	2.03	0.41
1:I:86:GLU:OE2	1:J:139:HIS:NE2	2.53	0.41
1:I:155:HIS:HA	1:I:159:ARG:NH1	2.36	0.41
1:A:3:PHE:O	1:A:4:GLN:O	2.38	0.41
1:E:56:LEU:HD11	1:E:106:SER:HB3	2.01	0.41
1:E:191:GLN:HA	1:E:192:PRO:HD3	1.93	0.41
1:E:225:CYS:HB3	1:G:95:ASN:OD1	2.20	0.41
1:G:56:LEU:HD23	1:G:79:ASN:O	2.21	0.41
1:I:29:LEU:HD23	1:I:111:PHE:CE2	2.51	0.41
1:C:46:GLN:OE1	1:C:66:LEU:HD12	2.21	0.41
1:C:123:ASN:C	1:C:124:THR:HG1	2.15	0.41
1:E:120:LEU:CD2	1:F:128:LEU:CD2	2.92	0.41
1:F:81:ARG:O	1:F:82:ASN:ND2	2.54	0.41
1:F:144:GLU:O	1:F:148:LEU:HG	2.20	0.41
1:C:207:ILE:HA	1:C:219:ASP:HB2	2.03	0.41
1:E:6:VAL:CG1	1:H:7:HIS:CE1	2.90	0.41
1:E:25:LEU:CD1	1:E:25:LEU:N	2.84	0.41
1:E:139:HIS:HB3	1:F:76:GLU:OE1	2.21	0.41
1:F:70:GLY:O	1:F:71:GLN:HB2	2.21	0.41
1:G:157:VAL:O	1:G:161:LEU:HG	2.21	0.41
1:H:34:LEU:HD12	1:H:108:LEU:O	2.20	0.41
1:H:179:VAL:O	1:H:180:ALA:C	2.63	0.41
1:I:8:GLN:HE22	1:I:25:LEU:CB	2.32	0.41
1:A:165:ALA:C	1:A:167:HIS:H	2.29	0.41
1:D:13:SER:O	1:D:137:ARG:NH2	2.54	0.41
1:H:166:ALA:O	1:H:167:HIS:HB2	2.21	0.41
1:J:84:PHE:O	1:J:85:ALA:CB	2.65	0.41
1:J:123:ASN:O	1:J:125:PRO:CD	2.68	0.41
1:G:50:ALA:HA	1:G:96:TYR:CZ	2.55	0.40
1:A:50:ALA:HA	1:A:96:TYR:CZ	2.56	0.40
1:B:153:ALA:O	1:B:157:VAL:HG23	2.21	0.40
1:B:225:CYS:O	1:B:226:PHE:O	2.39	0.40
1:G:155:HIS:HB3	1:G:187:HIS:HB2	2.01	0.40
1:G:187:HIS:O	1:G:188:LEU:HB2	2.20	0.40
1:H:15:HIS:CE1	1:H:16:LEU:HG	2.56	0.40
1:A:86:GLU:H	1:A:86:GLU:CD	2.29	0.40
1:A:122:ASP:O	1:A:123:ASN:HB2	2.22	0.40
1:A:191:GLN:HA	1:A:192:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:VAL:O	1:J:179:VAL:CG1	2.70	0.40
1:A:160:TYR:HE2	1:A:177:ILE:CD1	2.35	0.40
1:A:176:GLU:O	1:A:177:ILE:HB	2.20	0.40
1:A:225:CYS:SG	1:A:226:PHE:N	2.94	0.40
1:G:57:ILE:CD1	1:G:57:ILE:H	2.30	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	1:A:122:ASP:OD2[2_555]	1.58	0.62
1:C:210:LEU:CB	1:C:210:LEU:CD2[2_556]	1.76	0.44
1:H:69:GLU:OE2	1:I:79:ASN:OD1[4_456]	2.11	0.09

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	225/227 (99%)	197 (88%)	18 (8%)	10 (4%)	2 19
1	B	225/227 (99%)	202 (90%)	17 (8%)	6 (3%)	4 28
1	C	225/227 (99%)	183 (81%)	21 (9%)	21 (9%)	0 6
1	D	225/227 (99%)	189 (84%)	23 (10%)	13 (6%)	1 14
1	E	225/227 (99%)	197 (88%)	17 (8%)	11 (5%)	2 17
1	F	225/227 (99%)	193 (86%)	25 (11%)	7 (3%)	3 26
1	G	225/227 (99%)	197 (88%)	22 (10%)	6 (3%)	4 28
1	H	225/227 (99%)	195 (87%)	16 (7%)	14 (6%)	1 13
1	I	225/227 (99%)	207 (92%)	13 (6%)	5 (2%)	5 32
1	J	225/227 (99%)	198 (88%)	21 (9%)	6 (3%)	4 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2250/2270 (99%)	1958 (87%)	193 (9%)	99 (4%)	2 19

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	TYR
1	B	92	ASP
1	B	214	GLU
1	B	226	PHE
1	C	34	LEU
1	C	50	ALA
1	C	209	HIS
1	C	210	LEU
1	C	211	ASP
1	D	64	TYR
1	D	94	PRO
1	E	2	GLU
1	E	24	GLN
1	E	169	PRO
1	E	173	CYS
1	F	64	TYR
1	F	121	GLN
1	H	64	TYR
1	H	68	PRO
1	H	71	GLN
1	H	165	ALA
1	H	175	VAL
1	H	226	PHE
1	J	124	THR
1	A	4	GLN
1	A	176	GLU
1	B	70	GLY
1	C	123	ASN
1	C	213	ARG
1	C	214	GLU
1	D	166	ALA
1	D	190	ILE
1	F	188	LEU
1	G	64	TYR
1	G	178	PRO
1	H	70	GLY
1	H	169	PRO

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Mol	Chain	Res	Type
1	I	70	GLY
1	I	176	GLU
1	J	123	ASN
1	A	69	GLU
1	B	64	TYR
1	C	92	ASP
1	C	121	GLN
1	C	168	ALA
1	D	68	PRO
1	D	121	GLN
1	E	3	PHE
1	E	22	PRO
1	E	124	THR
1	H	69	GLU
1	J	175	VAL
1	A	5	ARG
1	A	122	ASP
1	A	181	LYS
1	B	177	ILE
1	C	35	VAL
1	C	189	SER
1	D	18	GLU
1	D	71	GLN
1	D	189	SER
1	E	123	ASN
1	F	51	HIS
1	F	125	PRO
1	G	4	GLN
1	I	175	VAL
1	J	4	GLN
1	A	105	PRO
1	C	66	LEU
1	C	69	GLU
1	C	71	GLN
1	D	74	ILE
1	D	104	VAL
1	E	168	ALA
1	E	178	PRO
1	F	69	GLU
1	H	66	LEU
1	H	176	GLU
1	H	191	GLN

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Mol	Chain	Res	Type
1	I	4	GLN
1	J	213	ARG
1	C	93	THR
1	C	208	ILE
1	D	52	ALA
1	D	69	GLU
1	G	105	PRO
1	G	123	ASN
1	H	105	PRO
1	A	125	PRO
1	C	125	PRO
1	C	177	ILE
1	I	178	PRO
1	H	67	THR
1	C	169	PRO
1	E	212	GLY
1	F	179	VAL
1	G	170	GLY
1	J	169	PRO
1	A	168	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	199/199 (100%)	192 (96%)	7 (4%)	31 60
1	B	199/199 (100%)	195 (98%)	4 (2%)	50 72
1	C	199/199 (100%)	191 (96%)	8 (4%)	27 56
1	D	199/199 (100%)	194 (98%)	5 (2%)	42 66
1	E	199/199 (100%)	197 (99%)	2 (1%)	73 85
1	F	199/199 (100%)	194 (98%)	5 (2%)	42 66
1	G	199/199 (100%)	193 (97%)	6 (3%)	36 63
1	H	199/199 (100%)	191 (96%)	8 (4%)	27 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	199/199 (100%)	197 (99%)	2 (1%)	73 85
1	J	199/199 (100%)	197 (99%)	2 (1%)	73 85
All	All	1990/1990 (100%)	1941 (98%)	49 (2%)	42 66

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PHE
1	A	4	GLN
1	A	57	ILE
1	A	90	PHE
1	A	108	LEU
1	A	128	LEU
1	A	138	LEU
1	B	57	ILE
1	B	67	THR
1	B	123	ASN
1	B	179	VAL
1	C	34	LEU
1	C	57	ILE
1	C	90	PHE
1	C	108	LEU
1	C	123	ASN
1	C	137	ARG
1	C	150	LEU
1	C	208	ILE
1	D	56	LEU
1	D	57	ILE
1	D	89	MET
1	D	90	PHE
1	D	188	LEU
1	E	119	GLN
1	E	208	ILE
1	F	37	LEU
1	F	57	ILE
1	F	108	LEU
1	F	183	LEU
1	F	215	ILE
1	G	57	ILE
1	G	67	THR
1	G	90	PHE

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Mol	Chain	Res	Type
1	G	108	LEU
1	G	177	ILE
1	G	183	LEU
1	H	57	ILE
1	H	82	ASN
1	H	95	ASN
1	H	108	LEU
1	H	118	ARG
1	H	162	LEU
1	H	183	LEU
1	H	184	VAL
1	I	75	LEU
1	I	160	TYR
1	J	120	LEU
1	J	171	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	95	ASN
1	A	107	GLN
1	A	155	HIS
1	B	9	GLN
1	B	12	GLN
1	B	26	GLN
1	B	107	GLN
1	C	12	GLN
1	C	121	GLN
1	C	123	ASN
1	C	200	HIS
1	D	7	HIS
1	D	79	ASN
1	D	95	ASN
1	D	123	ASN
1	E	14	HIS
1	E	15	HIS
1	E	95	ASN
1	E	107	GLN
1	E	119	GLN
1	E	187	HIS
1	E	200	HIS

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Mol	Chain	Res	Type
1	F	26	GLN
1	F	82	ASN
1	F	95	ASN
1	F	101	GLN
1	F	139	HIS
1	F	152	ASN
1	F	155	HIS
1	G	51	HIS
1	G	82	ASN
1	G	95	ASN
1	G	101	GLN
1	G	119	GLN
1	G	155	HIS
1	H	4	GLN
1	H	7	HIS
1	H	12	GLN
1	H	51	HIS
1	H	82	ASN
1	H	95	ASN
1	H	107	GLN
1	H	167	HIS
1	I	8	GLN
1	I	26	GLN
1	I	123	ASN
1	I	155	HIS
1	I	200	HIS
1	J	8	GLN
1	J	101	GLN
1	J	107	GLN
1	J	119	GLN
1	J	123	ASN
1	J	155	HIS
1	J	200	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	225/227 (99%)	0.31	9 (4%)	43	28	11, 51, 91, 100	47 (20%)
1	B	216/227 (95%)	0.42	5 (2%)	61	41	11, 50, 99, 100	70 (32%)
1	C	221/227 (97%)	0.43	11 (4%)	35	24	9, 50, 96, 100	57 (25%)
1	D	199/227 (87%)	0.28	6 (3%)	52	34	13, 47, 96, 100	66 (33%)
1	E	211/227 (92%)	0.48	9 (4%)	40	26	10, 56, 100, 100	75 (35%)
1	F	212/227 (93%)	0.46	6 (2%)	55	35	13, 57, 100, 100	76 (35%)
1	G	216/227 (95%)	0.35	9 (4%)	41	27	16, 59, 99, 100	66 (30%)
1	H	210/227 (92%)	0.39	5 (2%)	59	39	12, 55, 99, 100	54 (25%)
1	I	213/227 (93%)	0.45	10 (4%)	37	25	8, 55, 99, 100	46 (21%)
1	J	222/227 (97%)	0.51	10 (4%)	39	26	14, 63, 97, 100	43 (19%)
All	All	2145/2270 (94%)	0.41	80 (3%)	45	29	8, 55, 99, 100	600 (27%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	GLU	5.1
1	J	161	LEU	4.6
1	H	158	VAL	4.4
1	I	158	VAL	4.3
1	B	53	PHE	4.2
1	C	181	LYS	4.1
1	C	212	GLY	4.1
1	F	40	GLY	3.3
1	C	175	VAL	3.3
1	J	158	VAL	3.2
1	J	70	GLY	3.2
1	D	33	ASP	3.0
1	A	186	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	226	PHE	2.9
1	D	71	GLN	2.8
1	B	111	PHE	2.8
1	J	176	GLU	2.7
1	C	28	LEU	2.7
1	A	82	ASN	2.7
1	G	186	GLY	2.6
1	C	30	ALA	2.6
1	A	226	PHE	2.6
1	I	75	LEU	2.6
1	E	194	THR	2.5
1	I	159	ARG	2.5
1	E	206	GLY	2.5
1	A	227	GLU	2.5
1	I	16	LEU	2.5
1	E	157	VAL	2.5
1	H	71	GLN	2.5
1	I	53	PHE	2.4
1	I	49	PRO	2.4
1	I	180	ALA	2.4
1	C	188	LEU	2.4
1	B	215	ILE	2.4
1	G	100	ALA	2.4
1	E	188	LEU	2.4
1	F	55	TYR	2.4
1	G	187	HIS	2.4
1	J	33	ASP	2.4
1	F	153	ALA	2.3
1	H	165	ALA	2.3
1	J	38	ASP	2.3
1	G	175	VAL	2.3
1	A	187	HIS	2.3
1	J	206	GLY	2.3
1	E	140	GLN	2.3
1	G	166	ALA	2.2
1	J	219	ASP	2.2
1	C	37	LEU	2.2
1	C	1	MET	2.2
1	I	112	SER	2.2
1	G	203	GLY	2.2
1	A	54	TYR	2.2
1	E	35	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	196	SER	2.2
1	D	17	PHE	2.2
1	C	225	CYS	2.2
1	J	154	THR	2.2
1	I	163	THR	2.1
1	G	82	ASN	2.1
1	G	35	VAL	2.1
1	D	75	LEU	2.1
1	B	154	THR	2.1
1	A	208	ILE	2.1
1	J	223	LEU	2.1
1	H	124	THR	2.1
1	A	109	PHE	2.1
1	E	19	PRO	2.1
1	F	154	THR	2.1
1	C	176	GLU	2.1
1	D	16	LEU	2.1
1	H	204	ASP	2.1
1	F	11	LEU	2.1
1	I	182	GLN	2.0
1	B	56	LEU	2.0
1	F	189	SER	2.0
1	A	70	GLY	2.0
1	E	198	ILE	2.0
1	E	16	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.